

AD-762 476

**THERMAL ANALYSIS TESTING TO DETERMINE
THE COMPATIBILITY OF PROPELLANTS WITH
PLASTICS**

Frank D. Swanson, et al

Honeywell, Incorporated

AD 762 476

Prepared for:

Naval Ordnance Station

May 1973

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AD 762476

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Final Report

(May 23, 1972 To May 23, 1973)

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By

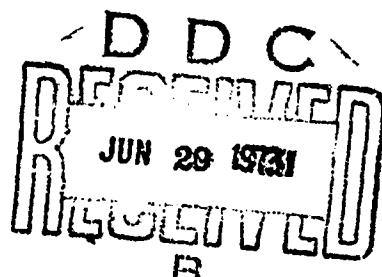
F. D. Swanson

J. L. Madsen

Prepared Under Contract N00174-72-C-0338

For

**Naval Ordnance Station
Indian Head, Maryland**



By

**Honeywell Inc.
Government And Aeronautical Products Division
600 Second Street North
Hopkins, Minnesota 55343**

DISTRIBUTION STATEMENT A
Approved for public release;
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UNCLASSIFIED

Security Classification

DOCUMENT CONTROL DATA - R & D

Security classification of title, body of abstract and indexing annotation must be entered when the overall report is classified)

1. ORIGINATING ACTIVITY (Corporate or firm) Honeywell Inc., Government and Aeronautical Products Division, 600 Second Street North Hopkins, Minnesota 55343		2a. REPORT SECURITY CLASSIFICATION Unclassified
		2b. GROUP NA
3. REPORT TITLE THERMAL ANALYSIS TESTING TO DETERMINE THE COMPATIBILITY OF PROPELLANTS WITH PLASTICS		
4. DESCRIPTIVE NOTES (Type of report and inclusive dates) Final Report - 23 May 1972 through 23 May 1973		
5. AUTHOR(S) (First name, middle initial, last name) Frank D. Swanson James L. Madsen		
6. REPORT DATE May 1973	7a. TOTAL NO. OF PAGES 61	7b. NO. OF REFS 13
8a. CONTRACT OR GRANT NO. N00174-72-C-0338	9a. ORIGINATOR'S REPORT NUMBER(S)	
b. PROJECT NO.		
c.	9b. OTHER REPORT NO(S) (Any other numbers that may be assigned this report)	
d.		
10. DISTRIBUTION STATEMENT Unlimited distribution.		
11. SUPPLEMENTARY NOTES	12. SPONSORING MILITARY ACTIVITY Naval Ordnance Station Indian Head, Maryland	
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UNCLASSIFIED

Security Classification

14 KEY WORDS	LINK A		LINK B		LINK C	
	ROLE	WT	ROLE	WT	ROLE	WT
Thermal Analysis Compatibility Propellants Plastics Differential Scanning Calorimetry Reaction Kinetics Computer-aided Analysis						

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1. INTRODUCTION

Recent developments in the field of polymer chemistry are being used increasingly in current munition design. Increased use of plastic materials is due to their fabrication flexibility, high strength-to-weight ratios, and low cost. However, in munitions, plastics are often used in direct contact with propellants or explosive materials. To ensure safety in handling and reliability after storage, plastic materials must be compatible with propellant materials.

Two aspects of compatibility must be considered. The plastic must not react with the propellant, creating a more sensitive or degraded product. Similarly, the propellant must not attack the plastic, resulting in degradation of the physical properties of the plastic. Thermal analysis is one of the analytical test techniques useful in evaluating the stability of a propellant exposed to a plastic material during the operational life of a munition.

The test program described in this report was performed using thermal analysis techniques to evaluate the compatibility of propellants M-26, PYRO and NACO with a variety of plastic adhesives and foams. The data generated give a statistical measure of propellant stability during aging in contact with the plastics. No data were generated regarding the effect of the propellant on the plastic materials.

II. SUMMARY

The objective of this program was to evaluate the stability of several propellants when aged in contact with plastic adhesives and foams. The data are required for application to Navy gun propulsion technology.

There are several tests useful in determining incompatibility in propellant-plastic mixtures. Rogers¹ has proposed the use of a thermal initiation test to determine short-term thermal instability. This technique is a modification of the older Henkin test². Long-term aging stability has been predicted principally by use of the vacuum stability test^{3, 4} that predicts compatibility by measuring gas evolution of the propellant-plastic system when aged at elevated temperatures. Variations of the vacuum stability test include Taliani, modified Taliani, and witness tests. These variations are primarily concerned with differences in recording and/or analyzing data.

The modified Henkin test is not useful for predicting long-term aging stability. The vacuum stability test will indicate short-term aging instability, although the results must be interpreted noting that typically only one test temperature is used. Several limitations should be noted concerning use of the vacuum stability test to determine long-term stability.

First, the test is not readily adaptable to quantitative analysis. In the typical vacuum stability test, as performed by Picatinny Arsenal⁴, a net increase of five milliliters in the amount of gas given off by five grams of propellant (due to exposure to the plastic) is considered evidence of excessive reactivity. The Naval Ordnance Laboratories have established four stability classes for the same test (see Table I). They determined each class by the volume of gas evolved per gram propellant after 48 hours at 100°C [(milliliters of gas measured at standard temperature and pressure (STP)].

Table I. Classification of Propellants by the 100°C Vacuum Stability Test⁵

Class	Milliliters of gas/gram/ 48 hours/STP	Quality
I	0-2	Satisfactory Stability
II	2-6	Borderline Stability
III	6-18	Unstable
IV	Over 18	Extremely Unstable, Possibly Hazardous

Evolution of additional gas* is attributed to undesirable interaction between the propellant and the plastic, or undesirable reactions induced by the polymer⁴. The gas evolution criterion, to be quantitatively useful, must be correlated with long-term aging tests on each propellant-plastic system. This, of course, is desirable regardless of the technique; still, it is not completely practical considering the large number of propellants and plastics available. To be of practical value, a test technique should yield data that will allow a kinetic analysis to predict aging stability.

The second limitation of the vacuum stability test is that the polymers are generally tested in the solid phase (thermoplastic or cured thermoset). In many end use applications, it is desirable to cure the plastic in contact with the propellant. This may create a system that is very unstable during cure of the polymer, but is compatible after the polymer is fully cured. This problem can be overcome by testing the vacuum stability of each of the plastic components (resin, curing agent, catalyst, filler, etc.) with the propellant and then testing the resulting cured system. Unfortunately, in some cases, this technique does not duplicate the environment experienced by the propellant, and it also markedly increases the test time.

Thermal analysis test techniques such as Differential Thermal Analysis (DTA), Differential Scanning Calorimetry (DSC), and Effluent Gas Analysis (EGA) can be used to determine short-term thermal instability and to predict long-term aging stability. Quantitative predictions of long-term aging stability can be made by applying one of several kinetic interpretations to the data. Both the fully cured polymer and the polymer curing against the propellant can be tested.

Thermal analysis techniques measure enthalpic effects attendant in most chemical or physical changes that occur within a material as the environmental temperature is increased at a selected rate. During a thermal analysis test, the temperature of the sample is compared with the temperature of a reference material while both are heated at a controlled rate. The results are normally plotted as temperature difference versus reference temperature. DSC combines the DTA method of temperature comparison with closed-loop heat compensation. The measurement plotted is the electrical energy in calories per second required to maintain the sample and reference at the same temperature. The results plotted show endothermic and exothermic peaks whose areas are directly proportional to the energy absorbed or liberated by the sample. EGA measures the relative quantity of gas evolved by the sample as the environmental temperature is increased at a selected rate.

*Additional gas refers to the quantity of gas evolved in excess of that evolved by propellant and plastic when separately exposed to 48 hours at 100°C.

In using thermal analysis to evaluate the compatibility of propellant-plastic combinations, the assumption is made that either sample temperature or gas evolution is maximum at the peak reaction rate. This assumption is well founded for propellants and explosives as indicated by Cook⁵.

III. DISCUSSION

Compatibility of the test plastics with various gun propellants was examined by thermal analysis techniques, primarily Differential Scanning Calorimetry.

Compatibility testing by thermal analysis examines the kinetics of the thermal decomposition reaction. The compatibility of a material is determined by the effect exposure to the material has on the decomposition reaction kinetics of the explosive or propellant.

It should be noted that these tests make no inferences as to the chemistry of the decomposition reaction or to the effect of the propellants on the test plastics.

Activation energy and frequency factor of the decomposition reaction were determined by the variable heating rate method as developed by Kissinger⁶ and modified by Pakulak⁷.

The reaction kinetics as described by Kissinger are based upon first order reaction rates. Assuming a first order reaction rate, an explosive will degrade as follows:

$$\left(\frac{\partial x}{\partial t} \right)_T = k_T (1-x) \quad (1)$$

where x = the fraction of the explosive degraded

t = time

k = the reaction rate constant at temperature (T).

The reaction rate constant is determined from the Arrhenius Rate Equation

$$k_{(T)} = A \exp (-E/RT) \quad (2)$$

where A = frequency factor

E = activation energy

R = gas constant (1. 987 calories/mole°K)

T = temperature in degrees Kelvin.

When the temperature is changing, as in a Differential Scanning Calorimeter run, the reaction rate becomes

$$\frac{dx}{dt} = \left(\frac{\partial x}{\partial t} \right)_T + \left(\frac{\partial x}{\partial T} \right)_t \frac{dT}{dt} \quad (3)$$

By determining X and T at the same instant, the time coordinate $\left(\frac{\partial x}{\partial t} \right)_t$ becomes zero. This reduces the rate equation to

$$\frac{dx}{dt} = A(1-x)\exp(-E/RT) \quad (4)$$

When the reaction is occurring at its maximum rate, its derivative with respect to time becomes zero. Solving for $\left(\frac{d}{dt} \right) \left(\frac{dx}{dt} \right)$, the equation becomes:

$$\frac{d}{dt} \left(\frac{dx}{dt} \right) = \frac{dx}{dt} \left(\frac{E}{RT^2} - \frac{dT}{dt} \right) = A \exp(-E/RT) \quad (5)$$

The temperature at which a reaction occurs at its maximum rate, dx/dt , can be measured as the peak exotherm temperature of a DSC thermogram. Therefore, the maximum reaction rate is defined as

$$A \exp(-E/RT_m) = \left(\frac{E}{RT_m^2} \right) \frac{dT}{dt} \quad (6)$$

where T_m is the peak temperature of a DSC trace. This equation reduces to the relationship

$$\frac{d \left(\ln \frac{\varphi}{T_m^2} \right)}{d \left(\frac{1}{T_m} \right)} = -\frac{E}{R} \quad (7)$$

where φ is the change in temperature with respect to time dT/dt or the sample heating rate.

The peak exotherms and heating rates from a series of DSC tests can be used to solve for the activation energy by Equation (7). Using this value for E, the frequency fact, A, can be determined by Equation (6). With the values of E and A determined, the rate constant, K, can be determined by using the Arrhenius Rate Equation, (2).

There are a number of assumptions necessary in making a prediction of kinetic data from thermal analysis data.

1. It is assumed that the decomposition by-products are a combination of gaseous and solid nonexplosive materials, free to escape without pressure buildup. An isothermal increase in pressure due to trapped gases would affect the decomposition reaction. It should be noted that the vacuum stability test is dependent on the formation of gaseous by-products for a prediction of stability. Thermal decomposition of explosives has been discussed by several authors, including Gray and Bonomo⁸ and Dacons, et al..
2. It is assumed that thermal decomposition values are comparable for the explosive in the melt, solid and vapor phases. This assumption is incorrect, but the difference in the decomposition rate for the two phases is not generally known. Various authors claim that the decomposition rates may be as much as 50 to 100 times faster in the melt phases than in the solid phases. For example, Gray and Bonomo⁹ have stated that production of TNT decomposition by-products is dependent on temperature, the greatest decomposition occurring between 150° and 160°F (the highest temperature studied in their work). The difference is, of course, due to the greater mobility of the atoms involved in the decomposition when the explosive is in the liquid phase (above its melting temperature). Several authors, including Farmer¹⁰ and Rosen¹¹, have discussed this area.

The techniques used for deriving the reaction kinetics from thermal analysis data are subject to much discussion. Reed, et al.¹² have argued that Kissinger's attempt to prove that the maximum reaction rate occurs at the peak of the DTA curve is incorrect. They note, additionally, that regardless of the proof, large errors in the calculated value of E can occur in systems when the maximum reaction rates are within 1°C (experimental error) of the peak temperature. Mastin¹³, in a theoretical study, has compared Kissinger's method with the modification used by Pakulak. In Kissinger's original method, the actual sample temperature at the peak differential temperature is used in Equation (7). The modified formula involves the use of the reference temperature at the maximum reaction rate. Mastin¹³ concludes that the Kissinger method will give reasonably good kinetic rate parameters in a simple decomposition reaction. He notes that the greatest error occurs at fast heating rates when it is assumed that the rate of change of the sample temperature at the maximum reaction rate is equal to the apparatus heating rate.

With a temperature-compensating design, as in the Perkin-Elmer DSC apparatus, this problem is diminished; however, thermal gradients within the sample are still a source of possible error. For this reason, sample sizes are kept to a minimum.

Given the processing conditions (the time at which the system will be held at the processing temperature), an arbitrary criterion can be established for short-term thermal stability. For example, such a criterion might require that the presence of test material with the explosive increase the amount of explosive reacted by less than one-tenth of one percent.

It is somewhat more difficult to establish a criterion for long-term aging stability because of the unknowns in storage time and temperature. In this case, a safe criterion would require that there be no significant increase in the decomposition rate due to the presence of the test material. This requirement dictates that the activation energy and frequency factor for the propellant only be compared with the same kinetic parameters for the propellant exposed to the plastic. Using the Arrhenius Rate Equation, predictions may be made as to the life of test and control samples. If these predictions are statistically similar, the system is compatible.

IV. TECHNICAL APPROACH

All testing was performed with a Perkin-Elmer model DSC-1B Differential Scanning Calorimeter. Sample preparation was as follows:

Samples weighing approximately 5 milligrams were cut from each of the propellants and run as controls. Then similar samples were run in contact with each of the various test plastics. With the liquid plastic samples, the propellant sample was coated and allowed to dry. With the solid and foam samples, the plastic was either cut into thin slices or ground to a powder and mixed with the propellant sample. The samples were placed into aluminum sample pans with an aluminum cover crimped over the top of the sample. The sample pans were placed in the DSC sample cells and covered with an aluminum dome. The temperature at which the decomposition rate reached its maximum, the peak exotherm on the DSC thermogram (Figure 1), was then recorded.

Due to nonlinearities in thermocouple output, the indicated temperature and the actual temperature of a DSC cell may not be the same across the entire temperature range of the instrument. Because of the need for precise temperature accuracy, it was necessary to calibrate the DSC apparatus. This was done by determining the indicated melt points of known standards across the entire temperature range and at each of the test heating rates. This operation was performed twice, first prior to the initial series of testing and again prior to a series of requested retests on some of the data. The calibration data is listed in Table II. The temperature correction data at each heating rate was found to be a second order curve. The coordinates of these curves were calculated to a least squares fit by computer and placed in a FORTRAN program that corrected the temperature error of the DSC runs and printed this data into data files. This program is listed in Appendix A as Corect-Temperature Correction Program.

The corrected data from each propellant and propellant-plastic combination was then run through a second FORTRAN program to calculate the activation energy, frequency factor, and reaction rate constant at any desired temperature. This program will also predict the extent of the decomposition reaction over any desired period of time at any desired temperature. This is an extrapolation of data over several magnitudes of time via an Arrhenius Rate Equation, which must be remembered when the predicted service lives are examined. This program is listed in Appendix A as Energy-Activation Energy Program.

One criterion for judging a plastic to be compatible with a propellant was that there be no statistically significant difference between the control and test sets of data. All statistical analysis was performed at 95 and 99 percent confidence levels.

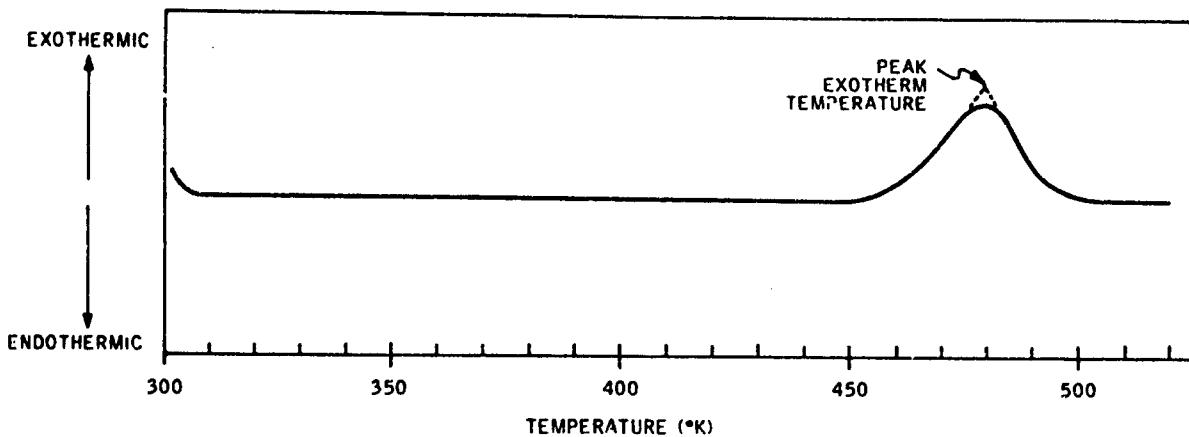


Figure 1. Typical DSC Thermogram

Table II. DSC Calibration

MATERIAL	TRUE MELT POINT (°K)	INDICATED MELT POINT (°K) AT HEATING RATE (°C/MINUTE) OF							
		80	40	20	10	5	2.5	1.25	
INITIAL TESTING - JULY 1972									
IODINE METAL	386.7	394.2	388.8	386.0	384.3	383.3	383.3		
INDIUM METAL	429.8	438.0	433.0	430.8	429.4	428.9	428.5		
AMMONIUM NITRATE	442.8	454.2	448.0	444.6	443.4	442.6	442.1		
EUTECTIC SOLDER	452.2	463.0	457.8	455.2	453.7	453.0	452.6		
TIN METAL	505.1	517.9	511.9	509.2	508.0	507.0	506.7		
LEAD	600.7	609.3	604.4	601.8	600.2	599.7	599.5		
RETESTING - FEBRUARY 1973									
NAPHTHALENE	353.4	354.2	348.6	346.2	345.0	344.3	343.4	343.5	
BENZOIC ACID	395.6	399.0	393.9	391.8	389.9	389.4	389.5	389.4	
INDIUM METAL	429.8	436.0	430.8	427.8	426.3	425.6	425.2	425.5	
2-CHLOROANTHRAQUINONE	482.1	489.1	483.0	481.4	480.2	479.4	479.4	479.8	
TIN METAL	505.1	512.8	507.4	504.8	503.3	502.7	502.2	502.9	
ANTHRAQUINONE	557.4	565.7	559.4	557.7	556.0	555.5	555.3	556.1	
LEAD	600.7	605.4	600.7	598.2	596.3	595.4	595.1	596.0	

The first test was an analysis to determine if the plot of $1/T$ versus $\log \phi/T^2$, from which the activation energy was calculated, was a fit to a straight line. This was done by the FORTRAN program listed in Appendix A as PROG1—Statistical Analysis - Program 1.

The second program, listed as PROG2—Statistical Analysis - Program 2, was used to compare the control and test data for each propellant-plastic combination. This program performed three tests. First, it determined if the variances in each data set were comparable. Second, it determined if the plots of $1/T$ versus $\log \phi/T^2$ for both the control and test sets of data were parallel. Third, it determined if the two plots were coincidental.

Each of these statistical programs must be satisfied in order that meaningful statements may be made regarding the compatibility of a given propellant-plastic combination.

The plot of $1/T$ versus $\log \phi/T^2$ measures the order of the reaction. If this plot fails to fit a straight line, the assumption that the reaction kinetics are first order is incorrect. None of the propellants evaluated failed this test.

Homogeneity of the sample variances is determined to test the assumption that the sample data comes from the same population. The statistical technique used to compare the parallelism and contingency of two sets of data (propellant only versus propellant-plastic combination) is dependent upon whether or not the variances are equal.

The condition of two sets of data being parallel determines whether or not exposure of the propellant to the plastic has significantly changed the activation energy of the propellant decomposition reaction. Under normal circumstances, the plastic will not change the activation energy of the propellant regardless of compatibility. When it occurs, a change in activation energy may indicate an incompatible propellant-plastic combination.

The condition of two sets of data being contingent determines whether exposure of the propellant to the plastic has significantly changed the frequency factor of the propellant decomposition reaction. Under normal circumstances, for a propellant-plastic combination that is not compatible the activation energy will not be changed (the lines will be parallel), but the frequency factor will be significantly increased (the lines will not be contingent). In the event of the frequency factor decreasing, it may be said that there is interaction between the plastic and propellant, but the result is not such that a degraded or hazardous propellant will result.

The results of the testing list any plastic-propellant combination that passed all of the tests as compatible. If a plastic-propellant combination failed at one confidence level and passed at the other, or failed any of the statistical tests at both confidence levels it was analyzed further by reviewing the shelf prediction obtained from the Arrhenius Rate Equation. Only in the case when a plastic-propellant combination failed the statistical tests and indicated a large change in shelf life was the system considered incompatible.

V. RESULTS AND CONCLUSIONS

The results of the DSC tests on each propellant and propellant-plastic combination are included in Appendix B. The temperatures listed are the corrected values. Included are the predictions for the percent of propellant unreacted when stored for 1, 2, 5, 10, and 20 years at 25°, 50°, 75°, and 100°C (298°, 323°, 348°, and 373°K). Also attached are the plots of $1/T$ versus Φ/T^2 for control and propellant-plastic combination.

Table III lists the results of the statistical analysis of the test data.

The data fits on NACO and PYRO control and plastic-propellant combinations were very good. The data for M-26 was much more scattered. For this reason, the limits for statistical noninteraction for M-26 tended to be quite broad, whereas the limits for the other propellants were more exacting. This accounts for the fact that some of the M-26 plastic combinations did not statistically interact, while their plots seemed to be more divergent than some of the other propellant-plastic combinations where statistical interaction was noted.

Several combinations are noted where statistical propellant-plastic interactions are noted. Reviewing the shelf-life predictions for each of these combination yields two examples of the plastic having a significant effect on the propellant. In each instance, the data would appear to suggest greater stability for the propellant due to exposure to the plastic. It is concluded that regardless of the effect predicted by extrapolation with the Arrhenius Rate Equation the systems have demonstrated a large chemical interaction that could be deleterious to device performance. For this reason M-26 with EC 1099 and PYRO with Ultrabond 76-125 are considered incompatible. In all other cases, the combinations are judged compatible.

Compatibility data was requested on Celcon 1011 with M-26 propellant. Considerable difficulty was experienced in attempting to achieve good DSC data due to melting of the Celcon prior to the decomposition of M-26. As an alternative approach, the Effluent Gas Analysis (EGA) accessory to the DSC was used in an attempt to determine the M-26 decomposition temperatures. EGA measures the relative quantities of gas output of a sample during a DSC run. Assuming that the peak decomposition temperature and the temperature at which peak gas evolution occurs are the same, EGA data should coincide with DSC data.

During the initial EGA testing with M-26 and Celcon, two problems were encountered. First, a short time lag exists between the evolution of the gas output of the sample and its detection by the EGA detector. This is due to time required for the gas to pass from the sample cell through a line to the EGA detector. Secondly, the EGA is presently set up to operate with nitrogen as a carrier gas. The use of a nitrogen atmosphere rather than air causes some changes in the decomposition characteristics of the M-26 propellant. These problems could be eliminated for future testing by careful calibration of the EGA time lag and conversion to air as a carrier gas.

Table III. Statistical Analysis Results

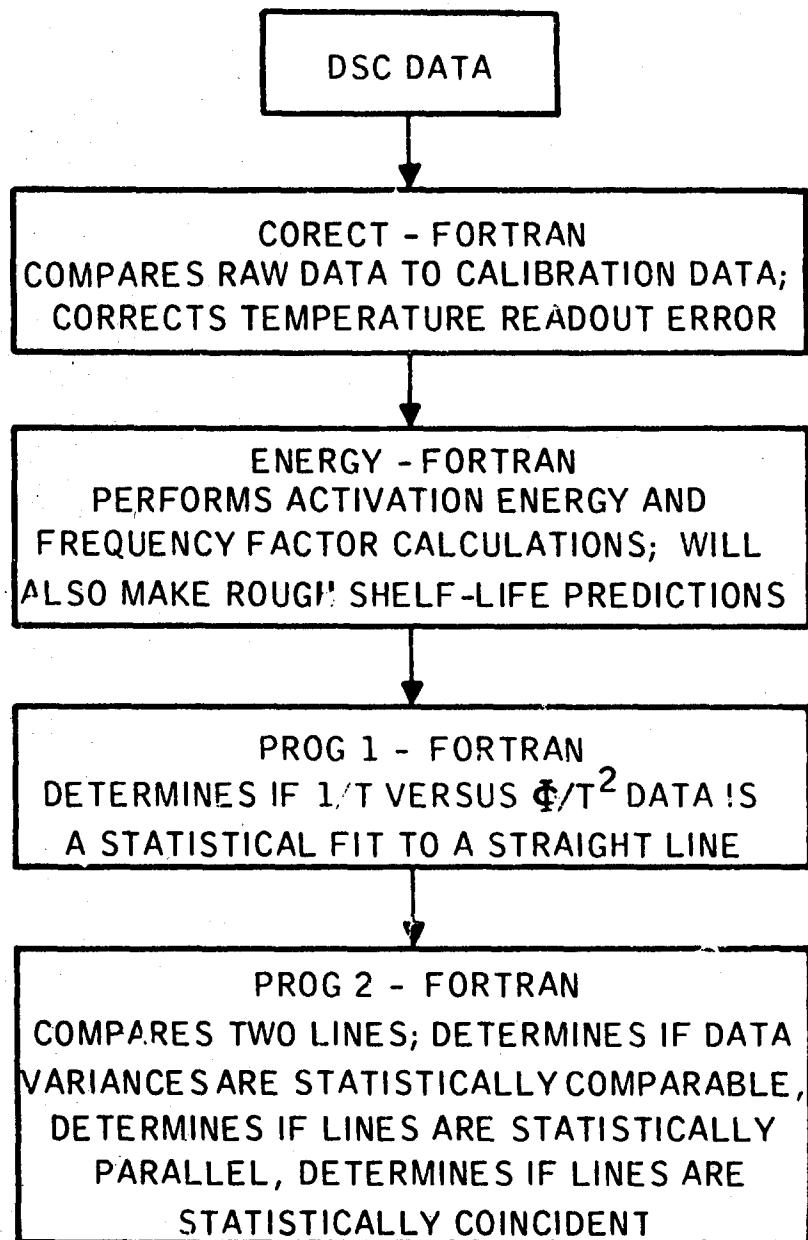
TEST SAMPLE	ACTIVATION ENERGY (KCAL/MOLE)	FREQUENCY FACTOR	PROG ONE	VARIANCES	PARALLEL	COINCIDENT	RATING
M-26 CONTROL	49.3	0.75×10^{21}	P	---	---	---	
M-26/GUN PLUG FOAM	53.9	0.11×10^{24}	P	P	P	P	COMPATIBLE
M-26/GUN PLUG FOAM (HUMIDITY)	54.6	0.27×10^{24}	P	P	P	P	COMPATIBLE
M-26/LOCTITE A	49.8	0.15×10^{22}	P	P	P	P	COMPATIBLE
M-26/LOCTITE N	47.4	0.10×10^{21}	P	P	P	P	COMPATIBLE
M-26/EC 1099	59.6	0.81×10^{26}	P	P	P	F	INCOMPATIBLE
M-26/UNFILLED CARTRIDGE CASE	49.7	0.10×10^{22}	P	P	P	P	COMPATIBLE
M-26/FILLED CARTRIDGE CASE	47.7	0.12×10^{21}	P	P	P	P	COMPATIBLE
PYRO CONTROL	44.4	0.19×10^{19}	P	---	---	---	
PYRO/UNFILLED CARTRIDGE CASE	45.8	0.93×10^{19}	P	P	M	M	COMPATIBLE
PYRO/FILLED CARTRIDGE CASE	44.6	0.26×10^{19}	P	P	P	P	COMPATIBLE
PYRO/ULTRABOND 76-125	52.6	0.20×10^{23}	P	P	M	M	INCOMPATIBLE
PYRO/EC 1099	46.6	0.25×10^{20}	P	P	P	F	COMPATIBLE
NACO CONTROL	47.4	0.64×10^{20}	P	---	---	---	
NACO/EC 1099	43.7	0.13×10^{19}	P	P	M	M	COMPATIBLE
NACO/ULTRABOND 76-125	44.6	0.36×10^{19}	P	P	P	P	COMPATIBLE

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APPENDIX A
COMPUTER PROGRAMS

Compatibility Analysis of Thermal Data



CORECT
FORTRAN -DSC TEMPERATURE CORRECTION

```
10 DIMENSION NAM(6),PARAM(8),A(3,8),P(8),TEMP(7),INDEX(25),T(25,7)
20 +,IFOR(14),MFOR(7)
30 DATA PARAM/80.,40.,20.,10.,5.,2.5,1.25,.625/,A/.358917E-3,
40 +.630512,83.0581,.302724E-3,.689625,73.1862,.294814E-3,.698029
50 +,73.7081,.32965E-3,.664192,83.1491,.296576E-3,.697677,75.5256
60 +,.293012E-3,.700064,75.5849,0.,1.,0.,0.,1.,0./
70 +,IFOR/'(I',4,'1H',',','F7','.3','7','(1','H','
80 +',F','7','.2'),')',MFOR/ '1','2','3','4','5','6','7'
90 WRITE(9,10)
100 10 FORMAT(/'NAME OF INPUT DATA FILE')
110 READ(9,20)NAM
120 20 FORMAT(6A2)
130 CALL DEFINE(1,NAM)
140 WRITE(9,30)
150 30 FORMAT(/'NAME OF DATA OUTPUT FILE')
160 READ(9,20)NAM
170 CALL DEFINE(2,NAM)
180 N=0
190 40 IF(IEOF(1).EQ.1)GOT0140
200 N=N+1
210 READ(1,50)LNO,P(N),TEMP
220 50 FORMAT(I5,8G10.0)
230 WRITE(9,60)P(N)
240 60 FORMAT(//'PHI:',F7.3//'MEASURED CALCULATED')
250 DO 70 I=1,8
260 IF(PARAM(I)-P(N))70,80,70
270 70 CONTINUE
280 STOP PHI NOT IN LIST
290 80 DO 90 J=1,7
300 IF(TEMP(J))100,100,90
310 90 CONTINUE
320 J=8
325 100 J=J-1
330 INDEX(N)=J
340 DO 120 K=1,J
350 T(N,K)=A(1,I)
360 DO 110 L=1,2
370 110 T(N,K)=T(N,K)*TEMP(K)+A(L+1,I)
380 120 WRITE(9,130)TEMP(K),T(N,K)
390 130 FORMAT(F8.2,F12.2)
400 GOT040
410 140 LNC=1
420 WRITE(2,150)LNO,N
430 150 FORMAT(I4,1H,,I4)
440 DO 160 I=1,N
450 LNO=LNO+1
460 J=INDEX(I)
470 IFOR(8)=MFOR(J)
480 160 WRITE(2,IFOR)LNO,P(I),(T(I,K),K=1,J)
490 STOP SAVE YOUR FILE
500 END
```

ENERGY
FORTRAN - ACTIVATION ENERGY PROGRAM

```
10 COMMON X(50,2),Y(50),A(2,2),U(7),C(50),T(9),AK(9),Z(9)
20 +, Q(9),B(2),DEG(9),NAM(6),AK1(9),EX(50),WYE(50)
30 DOUBLE PRECISION X,Y,A,C,AK,Q,B,YOU,DVEE,EO,E,R,D,ZEE
40 +,TEE,EFF,F,S1,S2,S3,EL,DF,P
50 COMPLEX RATIO
60 RATIO='INFINITE'
70 WRITE(9,10)
80 10 FORMAT(// 'WANT DATA FILE DESCRIPTION? (YES OR NO)')
90 READ(9,20)IWANT
100 20 FORMAT(6A2)
110 IF(IWANT.EQ.2HNO)GOTO40
120 WRITE(9,30)
130 30 FORMAT(// 'THIS PROGRAM FITS A 1-ST DEGREE POLYNOMIAL TO A BIVARI'
140 + 'ATE'// 'SET OF DATA, AND PRINTS A SUMMARY OF THE FIT.'// 'THE'
150 + ' DATA IS READ FROM A FILE WHICH MUST BE PREPARED PRIOR '
150 + 'TO EXECUTION.'// 'THE DATA FILE SHOULD BE SET UP AS FOLLOWS: //'
170 + 'LINE 1: LINE NO,M'// 'LINE 2: LINE NO,V1,U1,U2,U3,U4,U5,U6,U7'//
180 + 'LINE 3: LINE NO,V2,U1,U2,U3,U4,U5,U7'// '.....ETC'
190 + ' UNTIL ALL V-U DATA SETS HAVE BEEN ENTERED'// 'WHERE M IS '
200 + 'THE NUMBER OF V-U DATA SETS.'// 'VN IS A HEATING RATE IN '
210 + 'DEGREES C. PER MIN.'// 'AND EACH UN IS A TEMPERATURE IN DEGREES '
220 + 'KELVIN'// ' OBSERVED AT THE HEATING RATE VN.'/
230 + 'UP TO 7 TEMPERATURES MAY BE USED FOR 1 HEATING RATE.'/
240 + 'EACH LINE OF THE DATA FILE MUST BEGIN '
250 + 'WITH A LINE NUMBER'// 'FOLLOWED BY A COMMA.'// 'EACH ENTRY '
260 + 'EXCEPT THE LAST ON ANY LINE SHOULD BE FOLLOWED BY A COMMA.'// '
270 + 'FOLLOW THE ABOVE DATA WITH LINES CONTAINING'// '(IN ADDITION'
280 + ' TO THE LINE NUMBER):'/
290 + ' A) THE NUMBER OF STORAGE TEMPERATURES. (ZERO IF NONE.)'/
300 + ' *IGNORE STEPS B,C,D,AND E IF THE NUMBER ABOVE IS 0.**'/
310 + ' B) THE PARTICULAR STORAGE TEMPERATURES (DEGREES KELVIN)'/
320 + ' C) THE NUMBER OF VALUES FOLLOWING (ZERO IF NONE.)'/
330 + ' D) EITHER C1/C0 OR TIME, WHICHEVER IS TO BE SOLVED FOR.'/
340 + ' E) PARAMETER VALUES FOR TIME (YEARS), OR C1/C0 (PERCENT)'/
350 + ' -DEPENDING UPON WHAT WORD WAS TYPED FOR PART D.'// )
360 STOP
370 40 WRITE(9,50)
380 50 FORMAT(// 'NAME OF INPUT DATA FILE')
390 READ(9,20)NAM
400 CALL DEFINE(1,NAM)
410 WRITE(9,70)
420 70 FORMAT(// 'NAME OF OUTPUT DATA FILE')
430 READ(9,20)NAM
440 CALL DEFINE(2,NAM)
450 LNO=0
460 READ(1,80)LNS,M
470 80 FORMAT(2I6)
480 S3=0.00
490 WRITE(9,90)
500 90 FORMAT(// 'INPUT DATA'// ' PHI      TEMP'9X'I/I'1IX'PHI/ISQUARE')
```

ENERGY
FORTRAN - ACTIVATION ENERGY PROGRAM

```

10 COMMON X(50,2),Y(50),A(2,2),U(7),C(50),T(9),AK(9),Z(9)
20 +, Q(9),B(2),DEG(9),NAM(6),AKI(9),EX(50),WYE(50)
30 DOUBLE PRECISION X,Y,A,C,AK,Q,B,YOU,DVEE,E0,E,R,D,ZEE
40 +,TEE,EFF,F,S1,S2,S3,EL,DF,P
50 COMPLEX RATIO
60 RATIO='INFINITE'
70 WRITE(9,10)
80 10 FORMAT(// 'WANT DATA FILE DESCRIPTION? (YES OR NO)')
90 READ(9,20)IWANT
100 20 FORMAT(6A2)
110 IF(IWANT.EQ.2HNO)GOTO40
120 WRITE(9,30)
130 30 FORMAT(// 'THIS PROGRAM FITS A 1-ST DEGREE POLYNOMIAL TO A BIVARI'
140 + 'ATE'// 'SET OF DATA, AND PRINTS A SUMMARY OF THE FIT.'// 'THE'
150 + ' DATA IS READ FROM A FILE WHICH MUST BE PREPARED PRIOR '
160 + 'TO EXECUTION.'// 'THE DATA FILE SHOULD BE SET UP AS FOLLOWS:'// '
170 + 'LINE 1: LINE NO,M'// 'LINE 2: LINE NO,V1,U1,U2,U3,U4,U5,U6,U7'// '
180 + 'LINE 3: LINE NO,V2,U1,U2,U3,U4,U5,U6,U7'// '.....ETC'
190 + ' UNTIL ALL V-U DATA SETS HAVE BEEN ENTERED'// 'WHERE M IS '
200 + 'THE NUMBER OF V,U DATA SETS,'// 'VN IS A HEATING RATE IN '
210 + 'DEGREES C. PER MIN.,'// 'AND EACH UN IS A TEMPERATURE IN DEGREES '
220 + 'KELVIN'// ' OBSERVED AT THE HEATING RATE VN.'/
230 + 'UP TO 7 TEMPERATURES MAY BE USED FOR 1 HEATING RATE.'/
240 + 'EACH LINE OF THE DATA FILE MUST BEGIN '
250 + 'WITH A LINE NUMBER'// 'FOLLOWED BY A COMMA.'// 'EACH ENTRY '
260 + 'EXCEPT THE LAST ON ANY LINE SHOULD BE FOLLOWED BY A COMMA.'// '
270 + 'FOLLOW THE ABOVE DATA WITH LINES CONTAINING'// '(IN ADDITION'
280 + ' TO THE LINE NUMBER):'
290 + ' A) THE NUMBER OF STORAGE TEMPERATURES. (ZERO IF NONE.)'/
300 + ' *IGNORE STEPS B,C,D,AND E IF THE NUMBER ABOVE IS 0.**'/
310 + ' B) THE PARTICULAR STORAGE TEMPERATURES (DEGREES KELVIN)'/
320 + ' C) THE NUMBER OF VALUES FOLLOWING (ZERO IF NONE.)'/
330 + ' D) EITHER C1/CO OR TIME, WHICHEVER IS TO BE SOLVED FOR.'/
340 + ' E) PARAMETER VALUES FOR TIME (YEARS), OR C1/CO (PERCENT)'/
350 + ' -DEPENDING UPON WHAT WORD WAS TYPED FOR PART D.'// )
360 STOP
370 40 WRITE(9,50)
380 50 FORMAT(// 'NAME OF INPUT DATA FILE')
390 READ(9,20)NAM
400 CALL DEFINE(1,NAM)
410 WRITE(9,70)
420 70 FORMAT(// 'NAME OF OUTPUT DATA FILE')
430 READ(9,20)NAM
440 CALL DEFINE(2,NAM)
450 LNO=0
460 READ(1,80)LNS,M
470 80 FORMAT(2I6)
480 S3=0.D0
490 WRITE(9,90)
500 90 FORMAT(// 'INPUT DATA'// ' PHI      TEMP'9X'1/T'11X'PHI/TSQUARE')

```

ENERGY - PAGE 2

```
510 L=0
520 DO 130 I=1,M
530 READ(1,100)LNS,VEE,U
540 100 FORMAT(15,8E10.0)
550 DO 130 J=1,7
560 IF(U(J))130,130,110
570 110 L=L+1
580 EX(L)=1./U(J)
590 WYE(L)=VEE/(U(J)**2)
600 YOU=U(J)
610 DVEE=VEE
620 X(L,1)=1.00
630 X(L,2)=1.00/YOU
640 WRITIE(9,120)VEE,U(J),EX(L),WYE(L)
650 120 FORMAT(F7.2,F8.2,2E14.4)
660 Y(L)=DLOG(DVEE/(YOU**2))/DLOG(10.00)
670 WYE(L)=Y(L)
680 S3=S3+Y(L)**2
690 130 CONTINUE
700 LNO=LNO+1
710 WRITIE(2,140)LNO,L
720 140 FORMAT(14,1H,,14)
730 DO 150 I=1,L
740 LNO=LNO+1
750 150 WRITE(2,160)LNO,EX(I),WYE(I)
760 160 FORMAT(14,2(1H,,E14.6))
770 N=2
780 DO220 I=1,N
790 DO 200 J=1,N
800 A(I,J)=0.00
810 DO 180 K=1,L
820 180 A(I,J)=A(I,J)+X(K,I)*X(K,J)
830 IF (I.EQ.J) GOTO 200
840 LNO=LNO+1
850 AIJ=A(I,J)
860 WRITE (2,190)LNO,AIJ
870 190 FORMAT(14,1H,,E14.6)
880 200 CONTINUE
890 B(I)=0.00
900 DO 210 K=1,L
910 210 B(I)=B(I)+X(K,I)*Y(K)
920 LNO=LNO+1
930 BI=B(I)
940 220 WRITE (2,190)LNO,BI
950 LNO=LNO+1
960 ESS=S3
970 WRITE (2,190)LNO,ESS
980 DO 230 K=1,N
990 P=A(K,K)
1000 DO 230 J=K,N
1010 230 A(K,J)=A(K,J)/P
1020 B(K)=B(K)/P
1030 DO 250 I=1,N
1040 IF (I.EQ.K) GO TO 250
1050 F=A(I,K)
```

```

1060 DO 240 J=K,N
1070 240 A(I,J)=A(I,J)-F*A(K,J)
1080 B(I)=B(I)-F*B(K)
1090 250 CONTINUE
1100 WRITE(9,260)
1110 260 FORMAT( ///'LEAST SQUARES SOLUTION COEFFICIENTS ARE:'//)
1120 DO 280 I=1,N
1130 IM1=I-1
1140 BI=B(I)
1150 WRITE(9,270)IM1,BI
1160 270 FORMAT( '      A(' ,I3,') = ' ,E15.7)
1170 LNO=LNO+1
1180 280 WRITE (2,190)LNO,BI
1190 WRITE(9,290)
1200 290 FORMAT(//'POLYNOMIAL CURVE FIT OF DEGREE 1'//,
1210 + 3X'X-ACTUAL'7X'Y-ACTUAL'7X'Y-CALC'9X'DIFF'9X'PCT-DIFF'//)
1220 S1=0.00
1230 S2=0.00
1240 DO 330 I=1,L
1250 C(I)=B(N)*X(I,2)+B(N-1)
1260 D=Y(I)-C(I)
1270 S1=S1+D
1280 S2=S2+D*D
1290 CEE=C(I)
1300 DEE=D
1310 IF( C(I).EQ.0.00) GO TO 310
1320 OUT=100.00*D/C(I)
1330 WRITE(9,300)EX(I),WYE(I),CEE,DEE,OUT
1340 300 FORMAT(E13.6,3E15.6,F11.1)
1350 GOT0330
1360 310 WRITE(9,320)EX(I),WYE(I),CEE,DEE,RATIO
1370 320 FORMAT(E13.6,3E15.6,3X,4A2)
1380 330 CONTINUE
1390 EL=L
1400 EST=S1/EL
1410 WRITE(9,340)EST
1420 340 FORMAT(//'MEAN ERROR OF ESTIMATE FOR Y = ' ,E14.6)
1430 IF( L-2.NE.0)GOTO 360
1440 WRITE(9,350)
1450 350 FORMAT( 'NUMBER OF POINTS EQUALS DEGREE MINUS ONE'/
1460 + 'CURVE FIT IS SOLTUION OF SIMULTANEOUS EQUATIONS'/
1470 + 'STANDARD ERROR DOES NOT APPLY')
1480 GO TO 380
1490 360 DF=L-2
1500 STERR=DSQRT(S2/DF)
1510 WRITE(9,370)STERR
1520 370 FORMAT('UNBIASED STANDARD ERROR OF'//'ESTIMATE FOR Y: '
1530 +,16X,E14.6)
1540 LNO=LNO+1
1550 ESS=S2
1560 WRITE(2,190)LNO,ESS
1570 380 R=1.987D0
1580 E0=-DLOG(10.00)*R*B(2)*1.D-3
1590 E=-DLOG(10.00)*B(2)
1600 WRITE(9,390)

```

```

1610 390 FORMAT(//'"CALCULATED"/3X,'1/T      '7X'PHI/TSQUARE')
1620 DO 400 I=1,L
1630 F=DEXP(C(I)*DLOG(10.D0))
1640 IF(I.EQ.L)EFF=F
1650 FF=F
1660 400 WRITE(9,300)EX(I),FF
1670 D=DEXP(E*X(L,2))*EFF*E/60.D0
1680 EEO=E0
1690 DEE=D
1700 WRITE(9,410)EEO,DEE
1710 410 FORMAT(//'"E (KCAL/MOLE)"E14.6/"A (SEC-1)"      ,E13.6)
1720 READ(1,80)LNS,MO
1730 IF(MO.EQ.0)GOTO 580
1740 READ(1,100)LNS,(T(I),I=1,MO)
1750 DO 420 I=1,MO
1760 TEE=T(I)
1770 AK(I)=D*DEXP(-E/TEE)
1780 420 AKI(I)=AK(I)
1790 READ(1,80)LNS,M1
1800 IF(M1.EQ.0)GOTO540
1810 READ(1,430)LNS,VARY
1820 430 FORMAT(15,2A2)
1830 IF(VARY.NE.'TIME')WRITE(9,440)
1840 440 FORMAT(//'"DEGREES      K"8X"PER CENT, C1 OF CO, (TIME IN YEARS)"')
1850 IF(VARY.EQ.'TIME')WRITE(9,460)
1860 460 FORMAT(//'"DEGREES      K"8X"TIME IN MINUTES, (C1/CO IN PERCENT)"')
1870 470 FORMAT('KELVIN      (SEC -1)',6F8.1/)
1880 READ (1,100)LNS,(Z(J),J=1,M1)
1890 DO 490 J=1,M1
1900 ZEE=Z(J)
1910 IF(VARY.NE.'TIME') Q(J)=ZEE*365.D0*24.D0*3600.D0
1920 IF(VARY.EQ.'TIME') Q(J)=DLOG(100.D0/ZEE)/60.D0
1930 490 CONTINUE
1940 WRITE(9,470)(Z(J),J=1,M1)
1950 DO 520 I=1,MO
1960 DO 510 J=1,M1
1970 IF(VARY.EQ.'TIME')GOTO500
1980 F=Q(J)*AK(I)
1990 IF(F.GE.9.91)DEG(J)=0.
2000 IF(F.LT.9.91D0)DEG(J)=100.D0*DEXP(-F)
2010 GO TO 510
2020 500 DEG(J)=Q(J)/AK(I)
2030 510 CONTINUE
2040 520 WRITE(9,530)T(I),AKI(I),(DEG(J),J=1,M1)
2050 530 FORMAT(F7.1,E10.2,2X,6F8.2)
2060 GO TO 580
2070 540 WRITE(9,550)
2080 550 FORMAT('DEGREES      K'/'KELVIN      (SEC-1)')
2090 WRITE(9,560)(T(I),AKI(I),I=1,MO)
2100 560 FORMAT(4(F7.1,E10.2))
2110 580 WRITE(9,590)
2120 590 FORM:T(///'"<--> OUTPUT FILE")
2130 STOP
2140 END

```

PROGI
FORTRAN - STATISTICAL ANALYSIS - PROGRAM !

```
10 DIMENSION NAM(6)
20 COMMON X(30),Y(30),N,EN,SX(2),SY(2),SXY(2),A,B(2),XBAR,YBAR
25 DOUBLE PRECISION X,Y,EN,SX,SY,SXY,A,B,XBAR,YBAR
30 WRITE(9,10)
40 10 FORMAT('NAME OF INPUT DATA FILE')
50 READ(9,20)NAM
60 20 FORMAT(6A2)
70 CALL DEFINE(1,NAM)
80 WRITE(9,30)
90 30 FORMAT(1X, 'INPUT DATA'/4X'X',13X'Y')
100 READ(1,40)LNO,N
110 40 FORMAT(2I6)
170 DO 60 I=1,N
180 READ(1,50)LNO,X(I),Y(I)
190 50 FORMAT(16,3D20.0)
191 EX=X(I)
192 EY=Y(I)
193 60 WRITE(9,70)EX,EY
200 READ(1,50)LNO,SY(1)
205 READ(1,50)LNO,SX(1)
210 READ(1,50)LNO,SX(2)
215 READ(1,50)LNO,SXY(1)
220 READ(1,50)LNO,SY(2)
225 READ(1,50)LNO,B(1)
230 READ(1,50)LNO,B(2)
235 READ(1,50)LNO,SXY(2)
260 70 FORMAT(2E14.6)
270 EN=N
280 YBAR=SY(1)/EN
290 A=YBAR
300 XBAR=SX(1)/EN
310 SXY(2)=SXY(2)/(EN-2.DU)
312 SA=A
314 SB=B(2)
316 SXBAR=XBAR
320 WRITE(9,80)SA,SB,SXBAR
330 80 FORMAT('Y=A+B(X-XBAR)''/A:',E14.6/'B:',E14.6/'XBAR',E14.6)
341 IFRAT=1
342 90 FORMAT(16,2G10.0)
350 DO 95 I=1,2
352 READ(1,90)LNO,CL,F2
360 95 CALL INDEP(I,CL,F2,IFRAT)
361 DO 110 I=1,2
362 READ(1,100)LNO,CL,T,CHISQ1,CHISQ2
364 100 FORMAT(16,G10.0,3D10.0)
370 110 CALL CONLIM(I,CL,T,CHISQ1,CHISQ2)
380 STOP
390 END
1310 SUBROUTINE INDEP(I,CL,F,IFRAT)
1320 COMMON X(30),Y(30),N,EN,SX(2),SY(2),SXY(2),A,B(2),XBAR,YBAR
1325 DOUBLE PRECISION X,Y,EN,SX,SY,SXY,A,B,XBAR,YBAR
```

```

1330 DIMENSION SQS(3),IDF(3),DF(3),SQM(3)
1335 GOTO(5,35),I
1340 5 SQS(1)=(SXY(1)-SX(1)*SY(1)/EN)**2/(SX(2)-SX(1)**2/EN)
1350 IDF(1)=1
1360 DF(1)=IDF(1)
1370 SQM(1)=SQS(1)/DF(1)
1380 SQS(3)=SY(2)-SY(1)**2/EN
1390 IDF(3)=N-1
1400 SQS(2)=0.D0
1403 DO 7 IHOPE=1,N
1406 7 SQS(2)=SQS(2)+(Y(IHOPE)-(A+B(2)*(X(IHOPE)-XBAR)))**2
1410 IDF(2)=IDF(3)-IDF(1)
1420 DF(2)=IDF(2)
1430 SQM(2)=SQS(2)/DF(2)
1440 FRATIO=SQM(1)/SQM(2)
1450 WRITE(9,10)SQS(1),IDF(1),SQM(1),FRATIO
1460 10 FORMAT(/28HTEST FOR SLOPE EQUAL TO ZERO///38X,10HDEGREES OF/
1470 +23X49HSUM OF SQUARES  FREEDOM  MEAN SQUARE  F RATIO/
1480 +17HDUE TO REGRESSION 5X E14.6,I7,5X,E13.3,3X,F7.2)
1490 WRITE(9,20)SQS(2),IDF(2),SQM(2)
1500 20 FORMAT(8HRESIDUAL14XE14.6,I7,5X,E13.3)
1510 WRITE(9,30)SQS(3),IDF(3)
1520 30 FORMAT(/5HTOTAL17XE14.6,I7)
1530 35 WRITE(9,40)CL,IDF(1),IDF(2),F
1540 40 FORMAT(/2HATF5.1,12H % LEVEL AND,I3,1H,,I3,11H DEGREES OF
1550 +12H FREEDOM, F=F8.3)
1560 IF(FRATIO.GT.F)GOTO60
1565 IFRAT=IFRAT+1
1570 WRITE(9,50)
1580 50 FORMAT(40HF RATIO LESS THAN F, CONSEQUENTLY CANNOT)
1590 60 WRITE(9,70)
1600 70 FORMAT(47HACCEPT THE HYPOTHESIS THAT Y IS DEPENDENT ON X.)
1610 RETURN
1620 END
1630 SUBROUTINE CONLIM(J,CL,T,CHISQ1,CHISQ2)
1650 COMMON X(30),Y(30),N,EN,SX(2),SY(2),SXY(2),A,B(2),XBAR,YBAR
1655 DOUBLE PRECISION X,Y,EN,SX,SY,SXY,A,B,XBAR,YBAR,VAR(3),
1656 +SDEV(3),T,CHISQ1,CHISQ2,ACOEFF,BCOEFF,XCOEFF,SX2,YC
1657 GOTO(5,155),J
1660 5 VAR(1)=(SX(2)-SX(1)**2/EN)/(EN-1.D0)
1670 VAR(2)=(SY(2)-SY(1)**2/EN)/(EN-1.D0)
1680 VAR(3)=(EN-1.D0)*(VAR(2)-B(2)*B(2)*VAR(1))/(EN-2.D0)
1690 DO 10 I=1,3
1700 10 SDEV(I)=DSQRT(VAR(I))
1710 WRITE(9,120)N
1720 WRITE(9,130)XBAR,SDEV(1),VAR(1)
1730 WRITE(9,140)YBAR,SDEV(2),VAR(2)
1740 WRITE(9,150)SDEV(3),VAR(3)
1750 120 FORMAT(/11HSAMPLE SIZE,I4//12HESTIMATES OF/23X4HMEAN,10X
1760 +5HSIGMA,9X,13HSIGMA SQUARED)

```

PROGI - PAGE 3

```
1770 130 FORMAT(20HINDEPENDENT VARIABLE,3D14.6)
1780 140 FORMAT(18HDEPENDENT VARIABLE,2X,3D14.6)
1790 150 FORMAT(3HY,X,31X,2D14.6)
1800 155 ACOEFF=I*SDEV(3)/DSQRT(EN)
1810 ALOW=YBAR-ACOEFF
1820 AHIGH=YBAR+ACOEFF
1825 YB=YBAR
1830 WRITE(9,160)CL,ALOW,YB,AHIGH
1840 160 FORMAT(/F4.1,28H PER CENT CONFIDENCE LIMITS://9HPARAMETER,
1850 +13X,11HLOWER LIMIT,3X,9HESTIMATED5X11HUPPER LIMIT,/
1860 +16HINTERCEPT (YBAR),3X,3E14.6)
1870 BCOEFF=I*SDEV(3)/(SDEV(1)*DSQRT(EN-1.D0))
1880 BLOW=B(2)-BCOEFF
1890 BHIGH=B(2)+BCOEFF
1892 BEE=B(2)
1900 WRITE(9,170)BLOW,BEE,BHIGH
1910 170 FORMAT(5HSLOPE,14X,3E14.6)
1920 SYX2LO=VAR(3)/CHISQ1
1930 SYX2HI=VAR(3)/CHISQ2
1932 VARYX=VAR(3)
1940 WRITE(9,180)SYX2LO,VARYX,SYX2HI
1950 180 FORMAT(19HSIGMA SQUARED (Y.X)3E14.6)
1960 WRITE(9,190)CL
1970 190FORMAT(/F5.1,41H % CONFIDENCE LIMITS FOR MEAN OF Y VALUES
1980 +24H AT A PARTICULAR X VALUE//4X,1HX,13X,6HY CALC,8X,7HY UPPER
1990 +7X,7HY LOWER)
2000 ACOEFF=I*SDEV(3)
2100 SX2=SX(2)-SX(1)**2/EN
2110 DO 200 I=1,N
2120 XCOEFF=X(I)-XBAR
2121 YC=YBAR+B(2)*XCOEFF
2130 YC1=DEXP(YC*DLOG(10.D0))
2140 XCOEFF=DSQRT(1.D0/EN + XCOEFF**2/SX2)
2150 YC2=DEXP((YC+ACOEFF*XCOEFF)*DLOG(10.D0))
2160 YC3=DEXP((YC-ACOEFF*XCOEFF)*DLOG(10.D0))
2170 EX=X(I)
2180 200 WRITE(9,210)EX,YC1,YC2,YC3
2190 210 FORMAT(4E14.6)
2200 RETURN
2210 END
```

PROG2
STATISTICAL ANALYSIS - PROGRAM 2

```
10 DIMENSION NAM(6),N(3),IFRAT(2),ITRAT(2,2)
20 DOUBLE PRECISION EN(3),X(2,50),Y(2,50),SX(3,2),SY(3,2)
30 +,SXY(3,2),XBAR(3),YBAR(3),VARX(3),VARY(3),B(3,2),VARXY(3)
40 DO 10 I=1,3
50 N(I)=0
60 DO 10 J=1,2
70 SX(I,J)=0.
80 SY(I,J)=0.
90 10 SXY(I,J)=0.
100 IS=1
110 20 WRITE(9,30)IS
120 30 FORMAT(//23HNAME OF INPUT DATA FILE,I2)
130 READ(9,40)NAM
140 40 FORMAT(6A2)
150 CALL DEFINE(IS,NAM)
160 WRITE(9,50)
170 50 FORMAT(//1I1HINPUT DATA:/3X,1I1HINDEPENDENT,3X,9HDEPENDENT)
180 READ(IS,60)LNO,N(IS)
190 60 FORMAT(2I6)
200 NS=N(IS)
210 DO 70 I=1,NS
220 READ(IS,80)LNO,X(IS,I),Y(IS,I)
230 80 FORMAT(I6,3D20.0)
240 EX=X(IS,I)
250 EY=Y(IS,I)
260 70 WRITE(9,90)EX,EY
270 READ(IS,30)LNO,SY(IS,I)
280 READ(IS,30)LNO,SX(IS,1)
290 READ(IS,30)LNO,SX(IS,2)
300 READ(IS,80)LNO,SXY(IS,1)
310 READ(IS,80)LNO,SY(IS,2)
320 READ(IS,80)LNO,B(IS,1)
330 READ(IS,80)LNO,B(IS,2)
340 READ(IS,80)LNO,SXY(IS,2)
350 90 FORMAT(2E14.6)
360 IS=IS+1
370 IF(IS-2)20,20,100
380 100 DO 140 I=1,IS
390 GOTO(110,110,130),I
400 110 DO 120 J=1,2
410 SX(IS,I)=SX(IS,I)+SX(J,I)
420 120 SY(IS,I)=SY(IS,I)+SY(J,I)
430 N(IS)=N(IS)+N(I)
440 SXY(IS,I)=SXY(IS,I)+SXY(I,I)
450 130 EN(I)=N(I)
460 XBAR(I)=SX(I,I)/EN(I)
470 YBAR(I)=SY(I,I)/EN(I)
480 VARX(I)=SX(I,2)-SX(I,1)**2/EN(I)
490 VARY(I)=SY(I,2)-SY(I,1)**2/EN(I)
500 SXY(I,2)=SXY(I,I)-SX(I,1)*SY(I,1)/EN(I)
```

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510 B(1,2)=SXY(1,2)/VARX(1)
520 140VARXY(1)=(VARY(1)-B(1,2)**2*VARX(1))/(EN(1)-2.00)
530 EFF=VARXY(1)/VARXY(2)
540 IDF1=N(1)-2
550 IDF2=N(2)-2
560 WRITE(9,150)IDF1,IDF2,EFF
570 150FORMAT(/14,1H,,14,' DEGREES OF FREEDOM'//10.4,' F RATIO'//)
571 DO 180 I=1,2
572 READ (2,200)LNO,CL,F
573 IFRAT(I)=1
574 WRITE (9,160)CL,F
575 160FORMAT(F7.1,19H % CONFIDENCE LEVEL/
576 +,F7.3,24H VALUE OF F DISTRIBUTION)
577 IF(EFF.LE.F)GOTO180
578 IFRAT(I)=2
579 WRITE(9,170)
580 170 FORMAT(19HSIGNIFICANT, CANNOT )
581 180 WRITE(9,190)
582 190 FORMAT(44HACCEPT THE HYPOTHESIS THAT THE VARIANCES ARE
583 +6H EQUAL//)
584 IF((IFRAT(1).EQ.2).AND.(IFRAT(2).EQ.2))GOTO350
585 B1MB2=S(1,2)-B(2,2)
586 DF=N(1)+N(2)-4
587 NDF=DF
588 SYXP2=((EN(1)-2.00)*VARXY(1)+(EN(2)-2.00)*VARXY(2))/DF
589 VARBMB=SYXP2*(1.00/VARX(1)+1.00/VARX(2))
590 TEE=B1MB2/SQRT(VARBMB)
591 DO 290 I=1,2
592 READ(2,200)LNO,CL,T
593 200 FORMAT(16,3G10.0)
594 ITRAT(I,I)=1
595 IF(I.EQ.2)GOTO220
596 WRITE(9,210)NDF,TEE
597 210 FORMAT(/17,19H DEGREES OF FREEDOM/
598 +F7.3,22H VALUE OF T CALCULATED//)
599 220 IF(IFRAT(I).EQ.2)GOTO290
600 IF(ABS(TEE).GT.T)ITRAT(I,I)=2
601 WRITE(9,230)CL,T
602 230 FORMAT(/F7.1,19H % CONFIDENCE LEVEL
603 +/F7.3,33H ABSOLUTE VALUE OF T DISTRIBUTION)
604 IF(ITRAT(I,I).EQ.2)GOTO260
605 WRITE(9,250)
606 250 FORMAT(40HNON-SIGNIFICANT (THE LINES ARE PARALLEL)//)
607 GOTO290
608 260 WRITE(9,270)
609 270 FORMAT(40HSIGNIFICANT (THE LINES ARE NOT PARALLEL)//)
610 290 CONTINUE
611 IF((ITRAT(1,1).EQ.2).AND.(ITRAT(1,2).EQ.2))GOTO350
612 XVARPL=VARX(1)+VARX(2)
613 B(3,2)=(SXY(1,2)+SXY(2,2))/XVARPL
614 SXY140=VARY(1)+VARY(2)-B(3,2)*(SXY(1,2)+SXY(2,2))

```

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```
810 DF=N(1)+N(2)-3
820 NDF=DF
830 SYXP2=SXYTWO/DF
840 XBARMI=XBAR(1)-XBAR(2)
850 TEE=(YBAR(1)-YBAR(2)-B(3,2)*XBARMI)/SQRT(SYXP2*(1.D0/EN(1) +
860 +1.D0/EN(2) + XBARMI**2/XVARPL))
861 DO 340 I=1,2
370 READ(2,200)LN0,CL,T
871 ITRAT(2,I)=1
872 IF(I.EQ.2)GOT0295
873 WRITE(9,210)NDF,TEE
874 295 IF((IFRAT(I).EQ.2).OR.(ITRAT(1,I).EQ.2))GOT0340
875 IF(ABS(TEE).GT.T)ITRAT(2,I)=2
876 WRITE(9,230)CL,T
877 IF(ITRAT(2,I).EQ.2)GOT0320
900 WRITE(9,310)
910 310FORMAT(/47HNON-SIGNIFICANT (THE LINES CAN BE REGARDED AS A
920 +24H SINGLE COINCIDENT LINE))
930 GOT0340
940 320 WRITE(9,330)
950 330FORMAT(42HSIGNIFICANT (THE LINES ARE NOT COINCIDENT))
970 340 CONTINUE
980 350 STOP
990 END
```

APPENDIX B
DSC TEST DATA

M-26 CONTROL

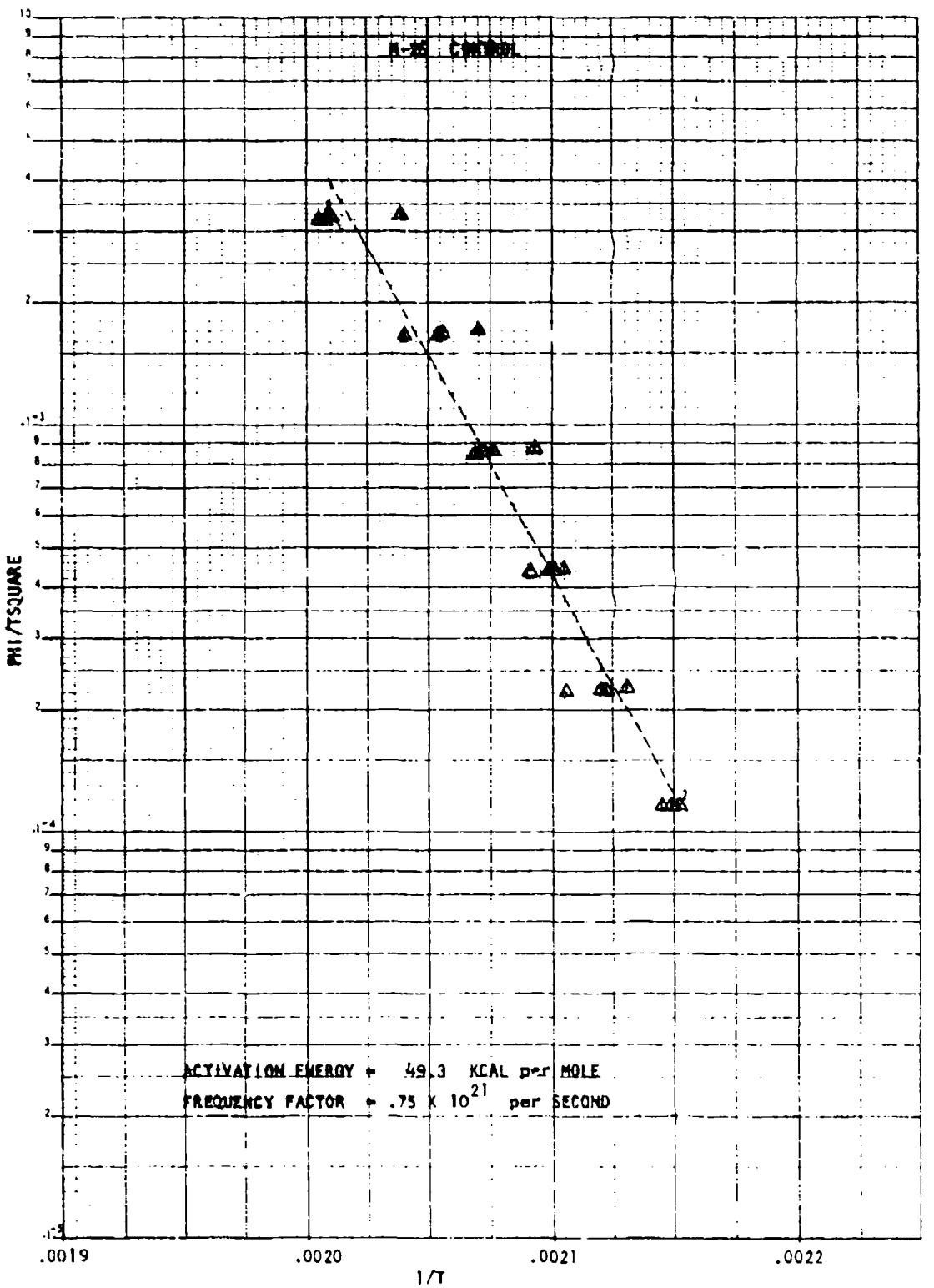
INPUT DATA

PHI	TEMP	1/T	PHI/ISQUARE
80.00	497.57	0.2010E-02	0.3231E-03
80.00	498.67	0.2005E-02	0.3217E-03
80.00	497.67	0.2009E-02	0.3230E-03
80.00	497.48	0.2010E-02	0.3233E-03
80.00	490.72	0.2038E-02	0.3322E-03
40.00	486.35	0.2056E-02	0.1691E-03
40.00	486.55	0.2055E-02	0.1690E-03
40.00	490.21	0.2040E-02	0.1665E-03
40.00	483.00	0.2070E-02	0.1715E-03
20.00	483.27	0.2069E-02	0.8563E-04
20.00	481.70	0.2076E-02	0.8619E-04
20.00	482.58	0.2072E-02	0.8588E-04
20.00	477.86	0.2093E-02	0.8758E-04
10.00	475.07	0.2105E-02	0.4431E-04
10.00	476.25	0.2100E-02	0.4409E-04
10.00	478.11	0.2092E-02	0.4375E-04
10.00	476.34	0.2099E-02	0.4407E-04
5.00	471.39	0.2121E-02	0.2250E-04
5.00	471.29	0.2122E-02	0.2251E-04
5.00	474.91	0.2106E-02	0.2217E-04
5.00	469.24	0.2131E-02	0.2271E-04
2.50	466.42	0.2144E-02	0.1149E-04
2.50	465.25	0.2149E-02	0.1155E-04
2.50	465.44	0.2149E-02	0.1154E-04
2.50	464.67	0.2152E-02	0.1158E-04

E (KCAL/MOLE) 0.492896E 02

A (SEC-1) 0.748259E 21

DEGREES KELVIN	K (SEC -1)	PERCENT, UNREACTED, (TIME IN YEARS)				
		1.0	2.0	5.0	10.0	20.0
298.0	0.53E-15	100.00	100.00	100.00	100.00	100.00
323.0	0.33E-12	100.00	100.00	99.99	99.99	99.98
348.0	0.83E-10	99.74	99.48	98.71	97.43	94.93
373.0	0.98E-08	73.39	53.86	21.29	4.53	0.21



M-26 / MK 12 GUN PLUG FOAM

INPUT DATA

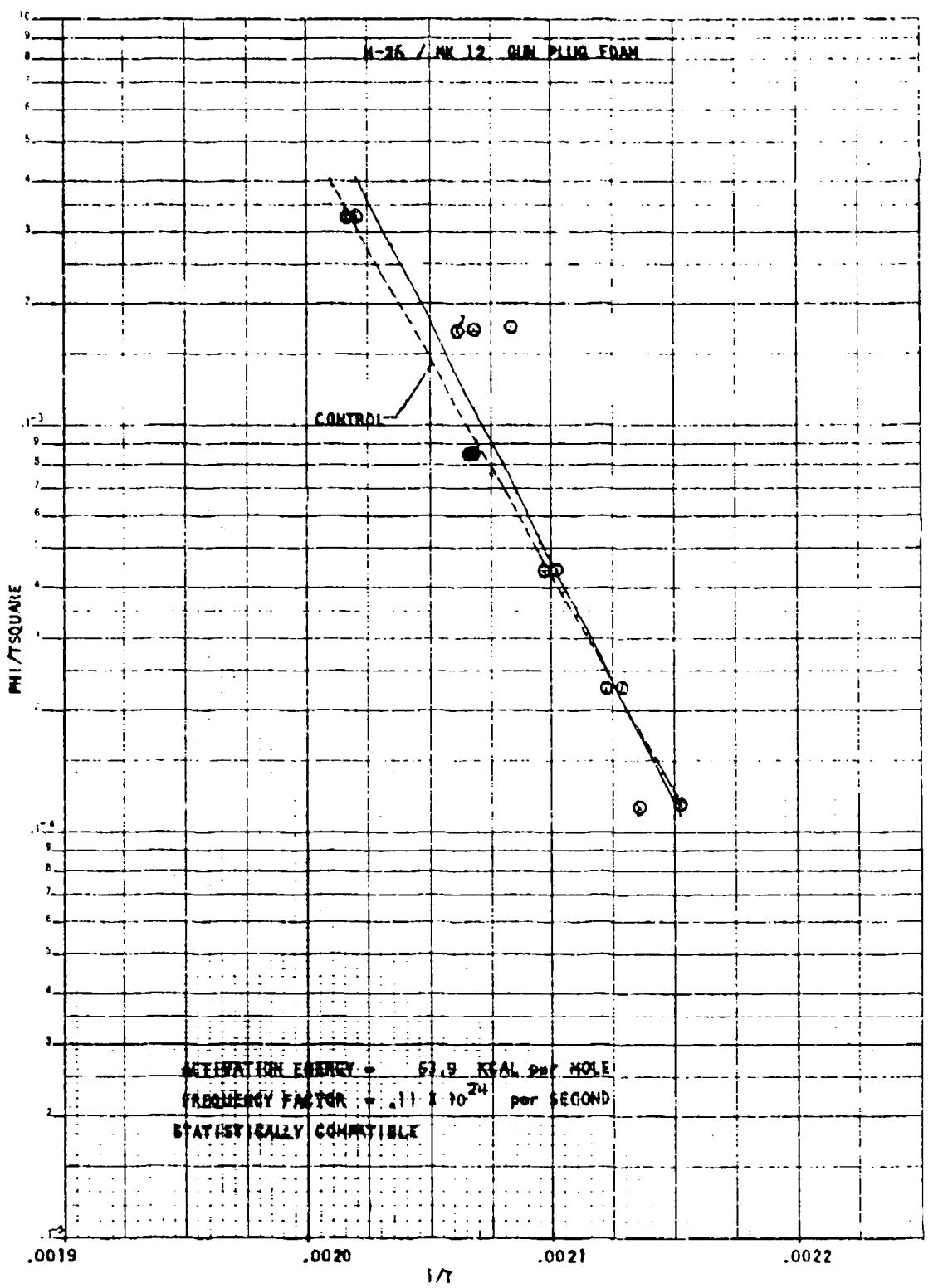
PHI	TEMP	1/T	PHI/TSQUARE
80.00	494.99	0.2020E-02	0.3265E-03
80.00	495.68	0.2017E-02	0.3256E-03
40.00	484.87	0.2062E-02	0.1701E-03
40.00	483.49	0.2068E-02	0.1711E-03
40.00	480.14	0.2083E-02	0.1735E-03
40.00	485.07	0.2062E-02	0.1700E-03
20.00	483.86	0.2067E-02	0.8543E-04
20.00	483.67	0.2068E-02	0.8549E-04
10.00	476.93	0.2097E-02	0.4396E-04
10.00	475.66	0.2102E-02	0.4420E-04
5.00	471.39	0.2121E-02	0.2250E-04
5.00	469.63	0.2129E-02	0.2267E-04
2.50	468.17	0.2136E-02	0.1141E-04
2.50	464.47	0.2153E-02	0.1159E-04

E (KCAL/MOLE) 0.538624E 02

A (SEC-1) 0.112227E 24

DEGREES K PERCENT, UNREACTED, (TIME IN YEARS)

KELVIN	(SEC -1)	1.0	2.0	5.0	10.0	20.0
298.0	0.00E 00	100.00	100.00	100.00	100.00	100.00
323.0	0.40E-13	100.00	100.00	100.00	100.00	100.00
343.0	0.17E-10	99.95	99.90	99.74	99.48	98.96
373.0	0.31E-08	90.75	82.36	61.55	37.89	14.36



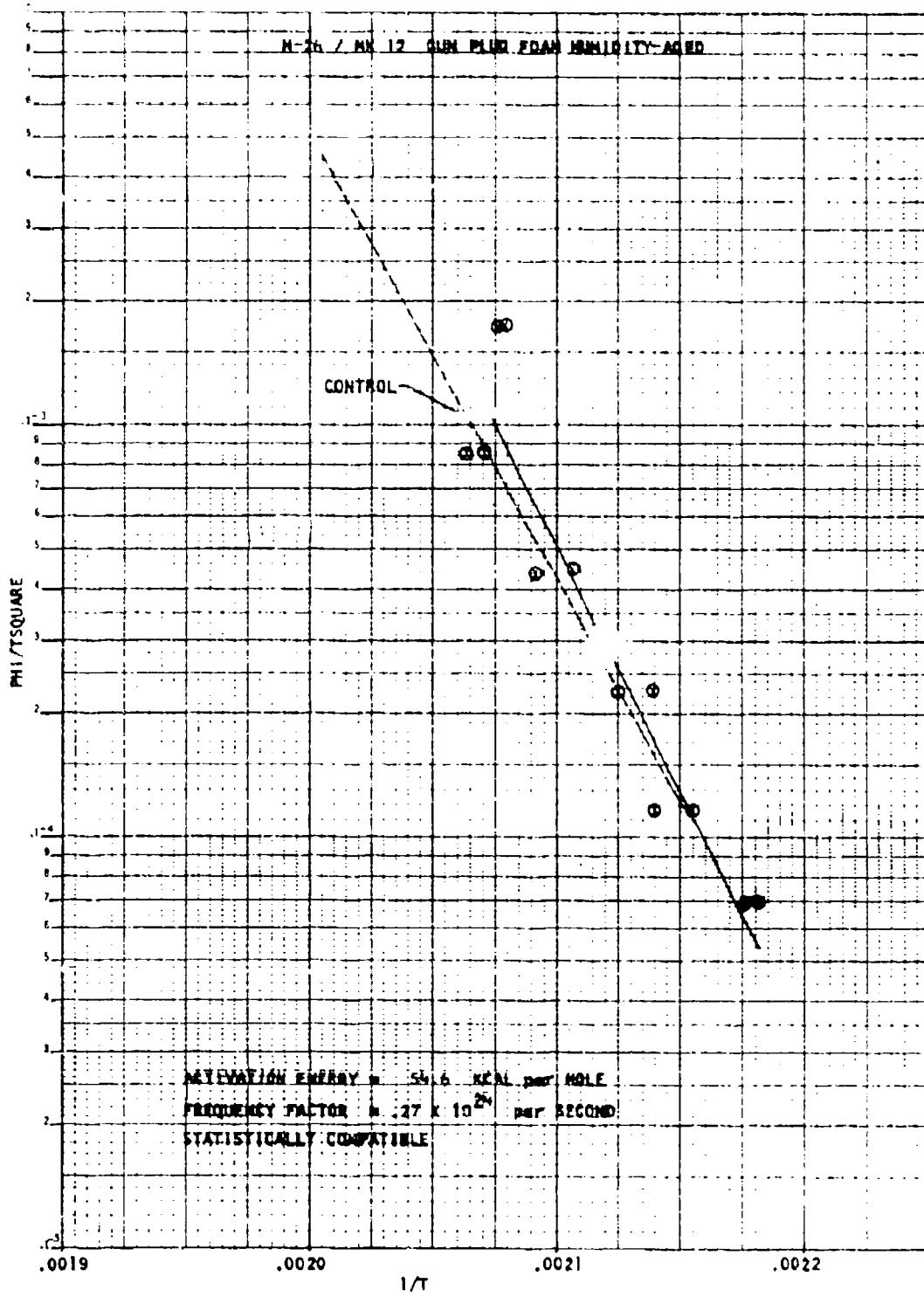
M-26 / MK 12 GUN PLUG FOAM,
HIMIDITY-AGED

INPUT DATA

PHI	TEMP	1/T	PHI/TSQUARE
40.00	481.08	0.2079E-02	0.1728E-03
40.00	481.57	0.2077E-02	0.1725E-03
20.00	484.44	0.2064E-02	0.8522E-04
20.00	482.95	0.2071E-02	0.8575E-04
10.00	477.93	0.2092E-02	0.4378E-04
10.00	474.50	0.2107E-02	0.4441E-04
5.00	467.67	0.2138E-02	0.2286E-04
5.00	470.60	0.2125E-02	0.2258E-04
2.50	467.34	0.2140E-02	0.1145E-04
2.50	463.93	0.2155E-02	0.1162E-04
1.25	459.32	0.2177E-02	0.5925E-05
1.25	458.35	0.2162E-02	0.5950E-05

E (KCAL/MOLE) 0.545899E 02
A (SEC-1) 0.265494E 24

DEGREES KELVIN	K (SEC -1)	PERCENT, UNREACTED, (TIME IN YEARS)					
		1.0	2.0	5.0	10.0	20.0	
298.0	0.00E 00	100.00	100.00	100.00	100.00	100.00	
323.0	0.30E-13	100.00	100.00	100.00	100.00	100.00	
348.0	0.14E-10	99.96	99.91	99.78	99.57	99.14	
373.0	0.27E-08	91.76	84.19	65.04	42.30	17.90	



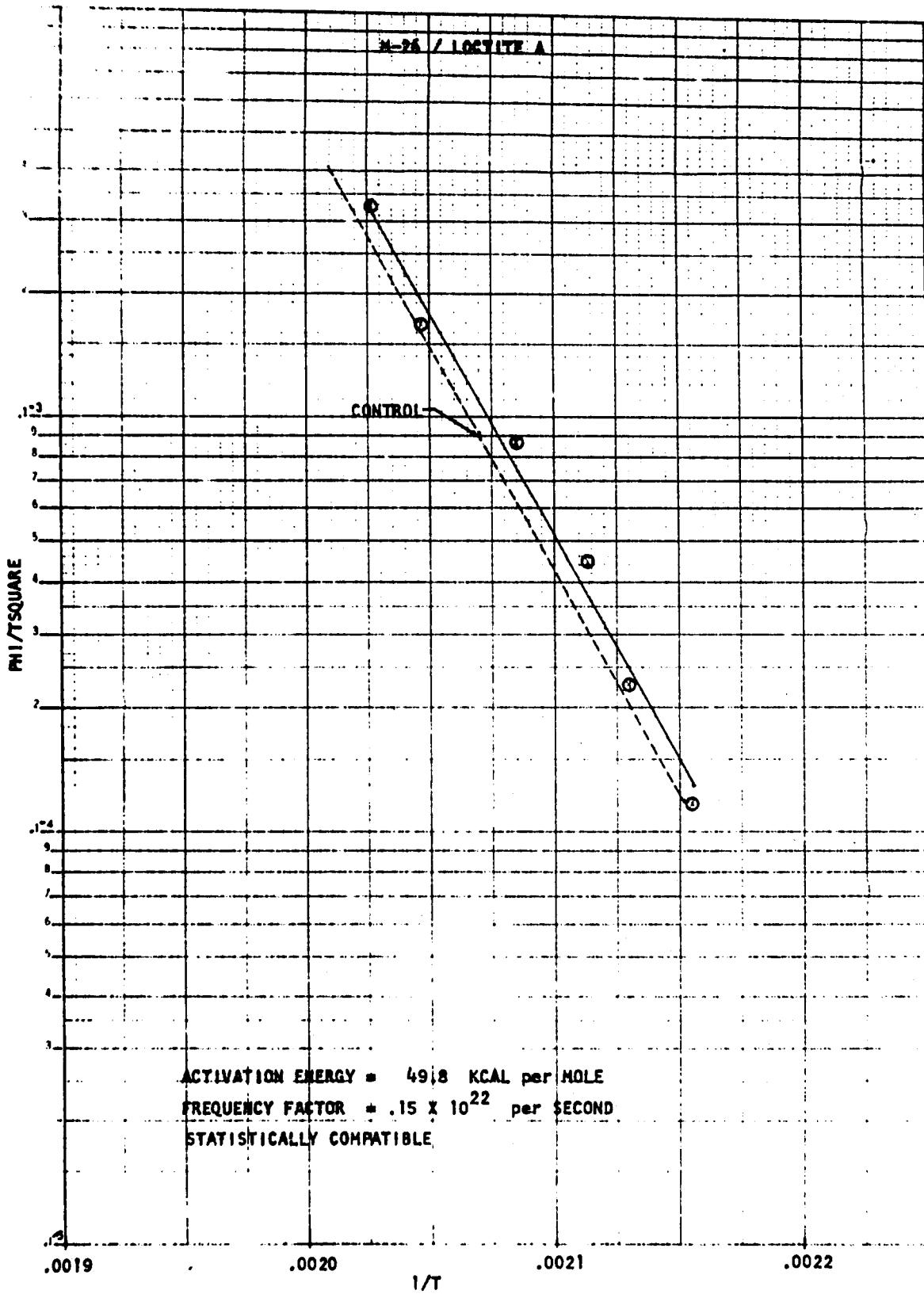
M-26 / LOCTITE A

INPUT DATA

PHI	TEMP	1/T	PHI/TSQUARE
80.00	493.50	0.2026E-02	0.3285E-03
40.00	488.53	0.2047E-02	0.1676E-03
20.00	479.73	0.2085E-02	0.8690E-04
10.00	473.12	0.2114E-02	0.4467E-04
5.00	469.53	0.2130E-02	0.2268E-04
2.50	463.98	0.2155E-02	0.1161E-04

E (KCAL/MOLE) 0.497688E 02
A (SEC-1) 0.150313E 22

DEGREES KELVIN	K (SEC -1)	PERCENT, UNREACTED, (TIME IN YEARS)				
		1.0	2.0	5.0	10.0	20.0
298.0	0.47E-15	100.00	100.00	100.00	100.00	100.00
323.0	0.32E-12	100.00	100.00	100.00	99.99	99.98
348.0	0.53E-10	99.74	99.48	98.70	97.42	94.90
373.0	0.10E-07	72.21	52.15	19.64	3.86	0.15



M-26 / LOCTITE N

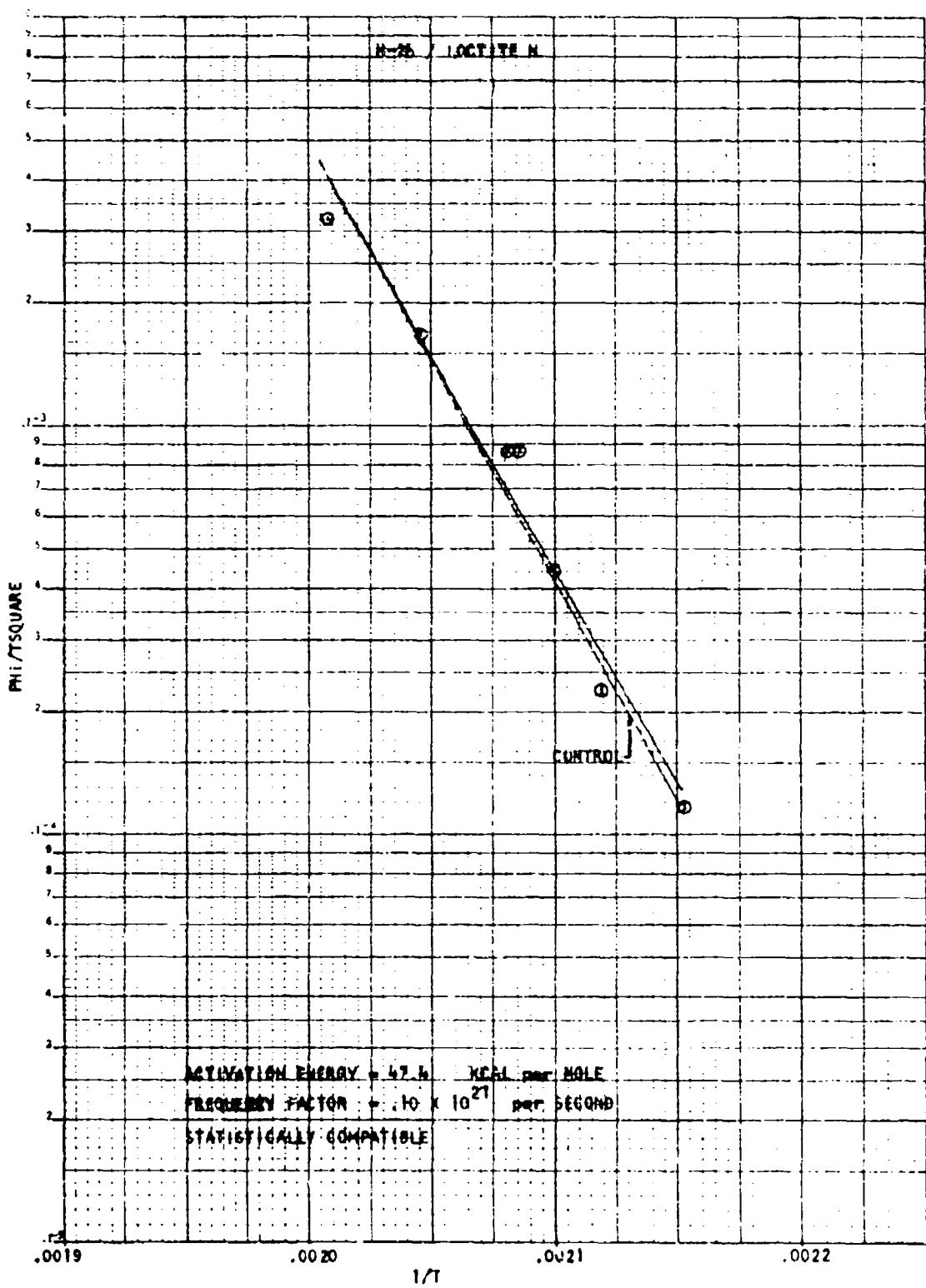
INPUT DATA

PHI	TEMP	1/T	PHI/TSQUARE
80.00	497.97	0.2008E-02	0.3226E-03
40.00	483.73	0.2046E-02	0.1675E-03
20.00	479.34	0.2086E-02	0.8704E-04
20.00	480.42	0.2082E-02	0.8665E-04
10.00	476.15	0.2100E-02	0.4411E-04
5.00	471.98	0.2119E-02	0.2245E-04
2.50	464.57	0.2153E-02	0.1158E-04

E (KCAL/MOLE) 0.474187E 02

A (SEC-1) 0.103894E 21

DEGREES KELVIN	K (SEC -1)	PERCENT, UNREACTED, (TIME IN YEARS)				
		1.0	2.0	5.0	10.0	20.0
298.0	0.17E-14	100.00	100.00	100.00	100.00	100.00
323.0	0.85E-12	100.00	99.99	99.99	99.97	99.95
348.0	0.17E-09	99.46	98.92	97.33	94.73	89.74
373.0	0.17E-07	58.50	34.22	6.85	0.47	0.00



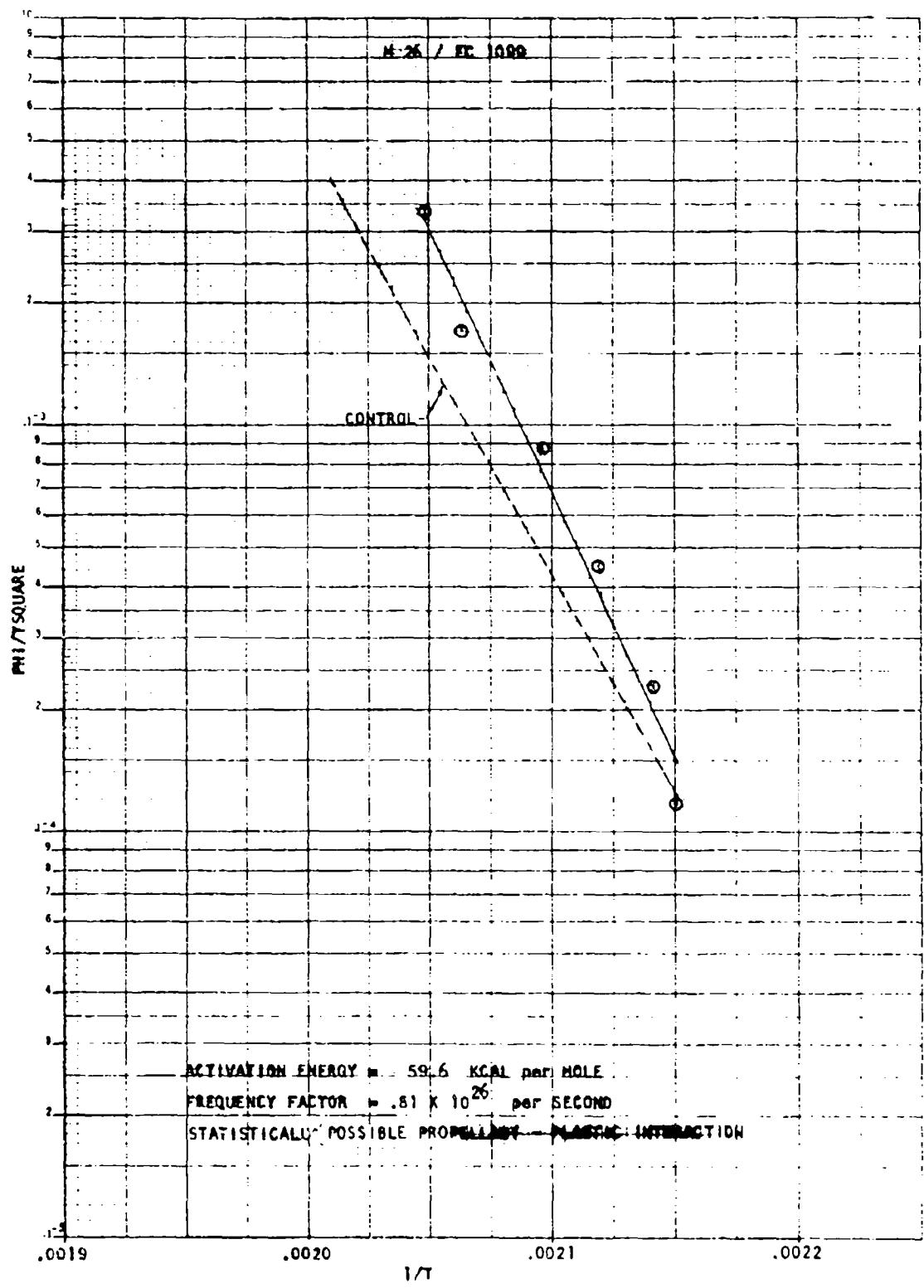
M-26 / EC 1099

INPUT DATA

PHI	TEMP	1/T	PHI/T ² SQUARE
80.00	488.04	0.2049E-02	0.3359E-03
40.00	484.77	0.2063E-02	0.1702E-03
20.00	477.08	0.2096E-02	0.8787E-04
10.00	471.85	0.2119E-02	0.4492E-04
5.00	467.00	0.2141E-02	0.2293E-04
2.50	464.96	0.2151E-02	0.1156E-04

E (KCAL/MOLE) 0.596298E 02
A (SEC-1) 0.806879E 26

DEGREES KELVIN	K (SEC -1)	PERCENT, UNREACTED, (TIME IN YEARS)				
		1.0	2.0	5.0	10.0	20.0
293.0	0.00E 00	100.00	100.00	100.00	100.00	100.00
323.0	0.00E 00	100.00	100.00	100.00	100.00	100.00
348.0	0.29E-11	99.99	99.98	99.96	99.91	99.82
373.0	0.92E-09	97.13	94.34	86.45	74.74	55.86



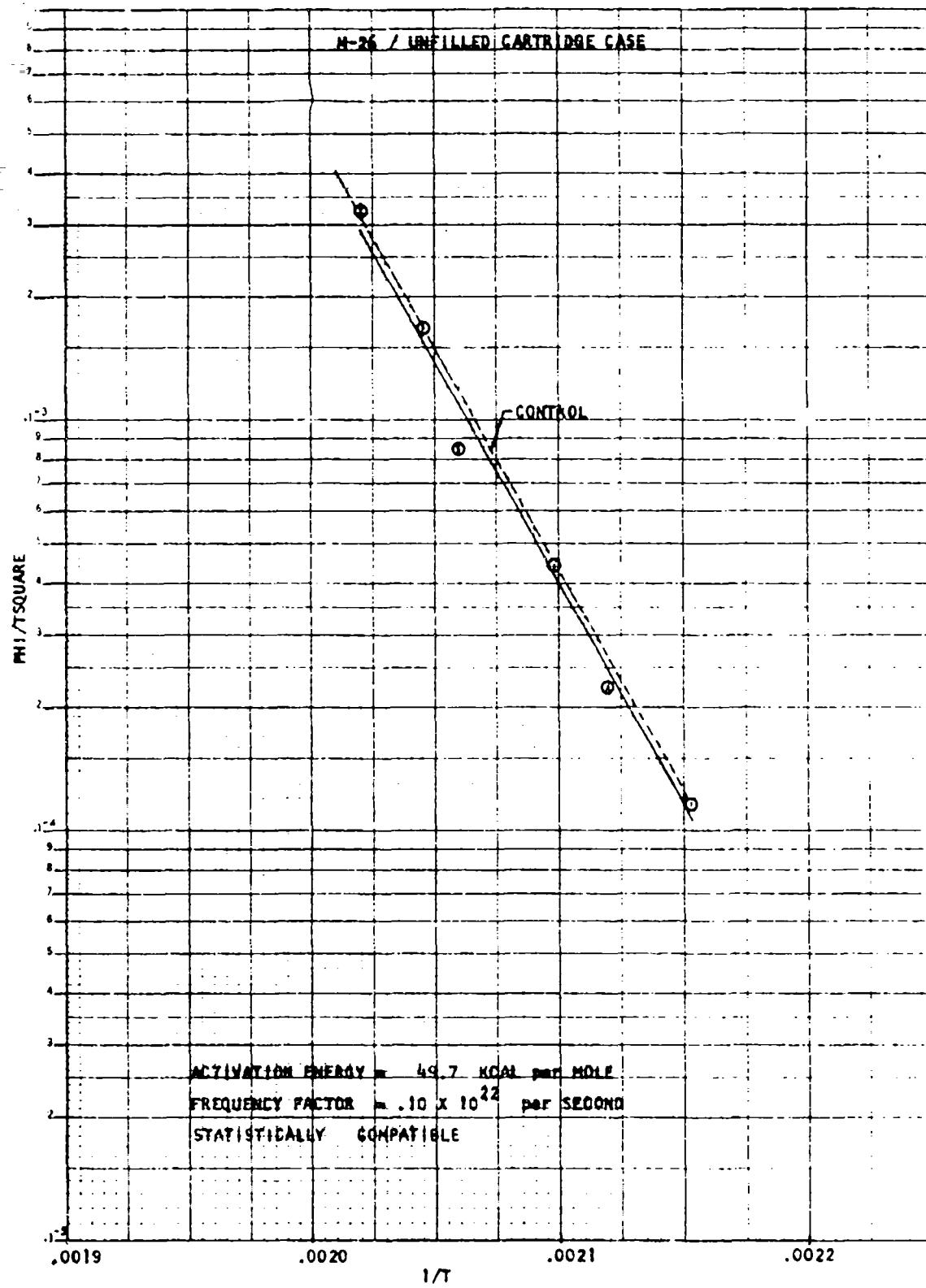
M-26 / UNFILLED CARTRIDGE CASE

INPUT DATA

PHI	TEMP	1/T	PHI/TSQUARE
80.00	494.99	0.2020E-02	0.3265E-03
40.00	488.73	0.2046E-02	0.1675E-03
20.00	485.64	0.2059E-02	0.8480E-04
10.00	476.54	0.2098E-02	0.4404E-04
5.00	471.88	0.2119E-02	0.2245E-04
2.50	464.47	0.2153E-02	0.1159E-04

E (KCAL/MOLE) 0.496687E 02
A (SEC-1) 0.103975E 22

DEGREES KELVIN	K (SEC -1)	PERCENT, UNREACTIONED, (TIME IN YEARS)				
		1.0	2.0	5.0	10.0	20.0
298.0	0.39E-15	100.00	100.00	100.00	100.00	100.00
323.0	0.26E-12	100.00	100.00	100.00	99.99	99.98
348.0	0.66E-10	99.79	99.58	98.96	97.93	95.90
373.0	0.82E-08	77.28	59.72	27.56	7.60	0.58



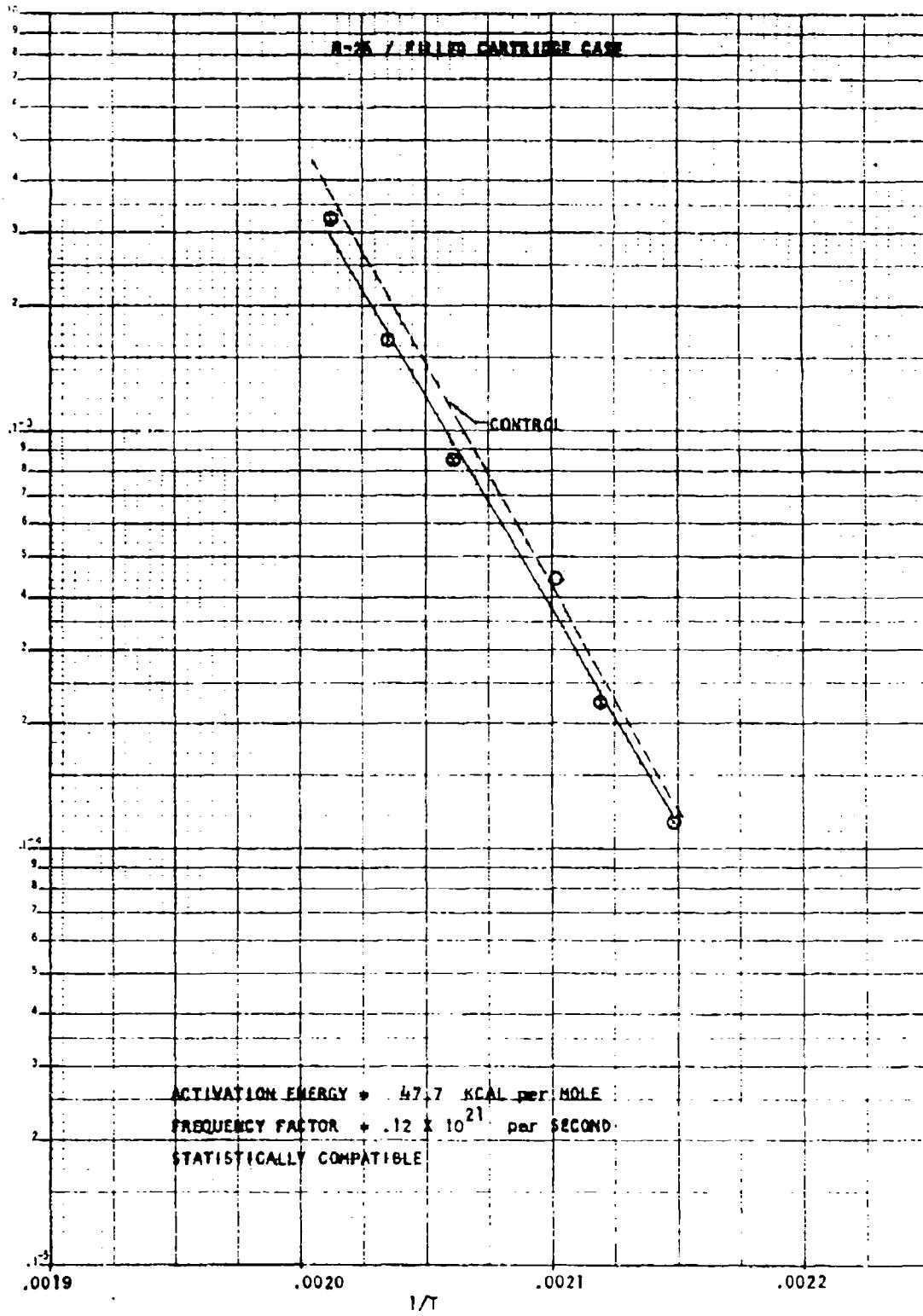
M-26 / FILLED CARTRIDGE CASE

INPUT DATA

PHI	TEMP	1/T	PHI/TSQUARE
80.00	496.98	0.2012E-02	0.3239E-03
40.00	491.50	0.2035E-02	0.1656E-03
20.00	485.15	0.2061E-02	0.8497E-04
20.00	484.95	0.2062E-02	0.8504E-04
5.00	471.78	0.2120E-02	0.2246E-04
2.50	465.44	0.2149E-02	0.1154E-04

E (KCAL/MOLE) 0.477363E 02
A (SEC-1) 0.116241E 21

DEGREES KELVIN	K (SEC -1)	PERCENT, UNREACTED, (TIME IN YEARS)				
		1.0	2.0	5.0	10.0	20.0
298.0	0.11E-14	100.00	100.00	100.00	100.00	100.00
323.0	0.58E-12	100.00	100.00	99.99	99.98	99.96
348.0	0.12E-09	99.62	99.24	98.11	96.25	92.64
373.0	0.12E-07	67.65	45.76	14.17	2.01	0.04



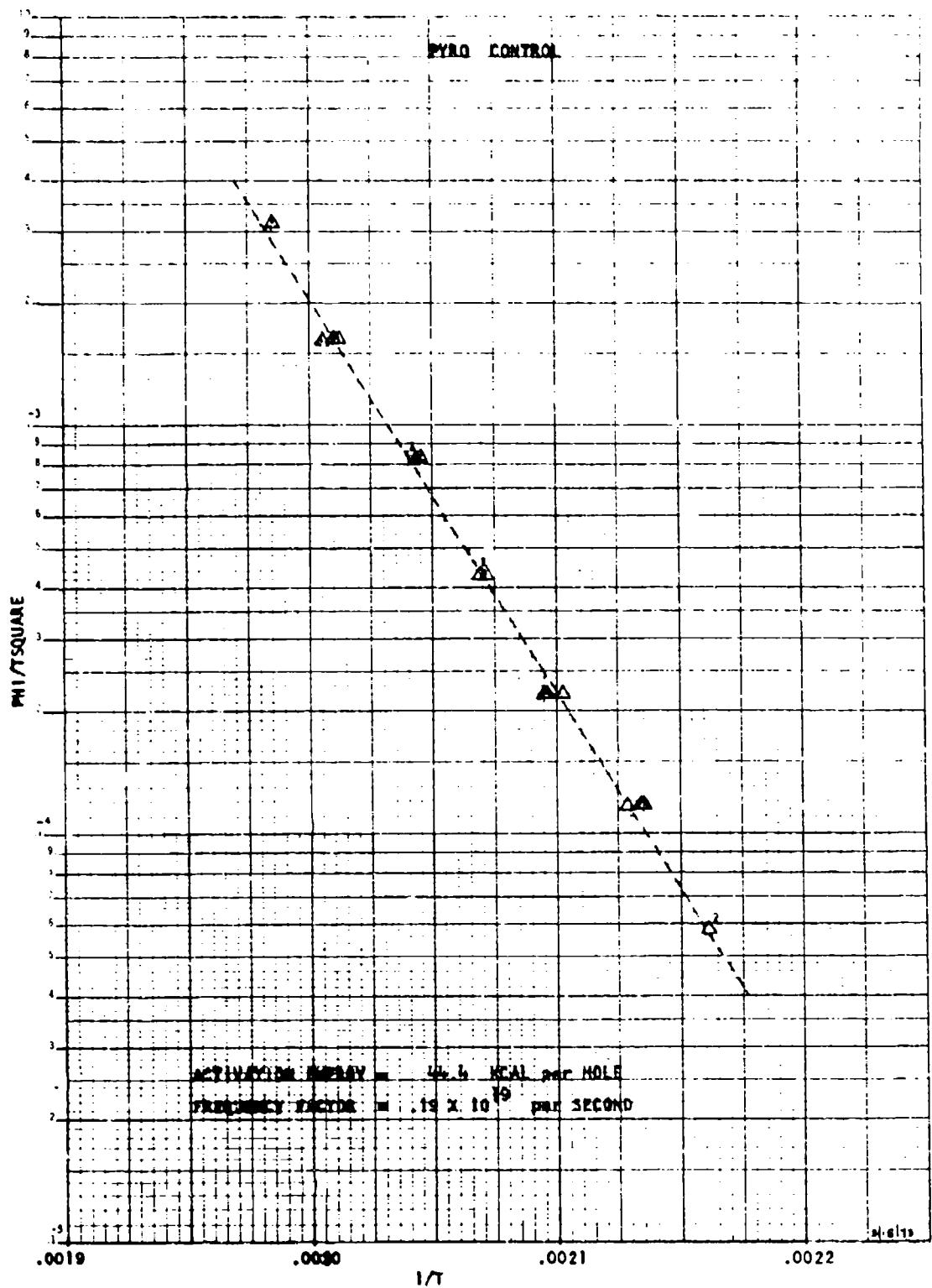
PYRO CONTROL

INPUT DATA

PHI	TEMP	I/T	PHI/TSQUARE
80.00	503.47	0.1986E-02	0.3156E-03
40.00	496.90	0.2012E-02	0.1620E-03
40.00	498.39	0.2006E-02	0.1610E-03
40.00	497.45	0.2010E-02	0.1616E-03
20.00	488.93	0.2045E-02	0.8366E-04
20.00	489.43	0.2043E-02	0.8349E-04
20.00	489.49	0.2043E-02	0.8347E-04
10.00	482.86	0.2071E-02	0.4289E-04
10.00	482.86	0.2071E-02	0.4289E-04
10.00	483.32	0.2069E-02	0.4281E-04
5.00	476.98	0.2097E-02	0.2198E-04
5.00	477.48	0.2094E-02	0.2193E-04
5.00	475.80	0.2102E-02	0.2209E-04
2.50	468.81	0.2133E-02	0.1137E-04
2.50	468.32	0.2135E-02	0.1140E-04
2.50	469.93	0.2128E-02	0.1132E-04
1.25	462.71	0.2161E-02	0.5838E-05
1.25	462.71	0.2161E-02	0.5838E-05

E (KCAL/MOLE) 0.443645E 02
 A (SEC-1) 0.193012E 19

DEGREES KELVIN	K (SEC -1)	PERCENT, UNREACTED, (TIME IN YEARS)					
		1.0	2.0	5.0	10.0	20.0	
298.0	0.56E-14	100.00	100.00	100.00	100.00	100.00	
323.0	0.18E-11	99.99	99.99	99.97	99.94	99.83	
348.0	0.26E-09	99.17	98.35	95.92	92.01	84.66	
373.0	0.19E-07	54.13	29.30	4.65	0.22	0.00	



PYRO / UNFILLED CARTRIDGE CASE

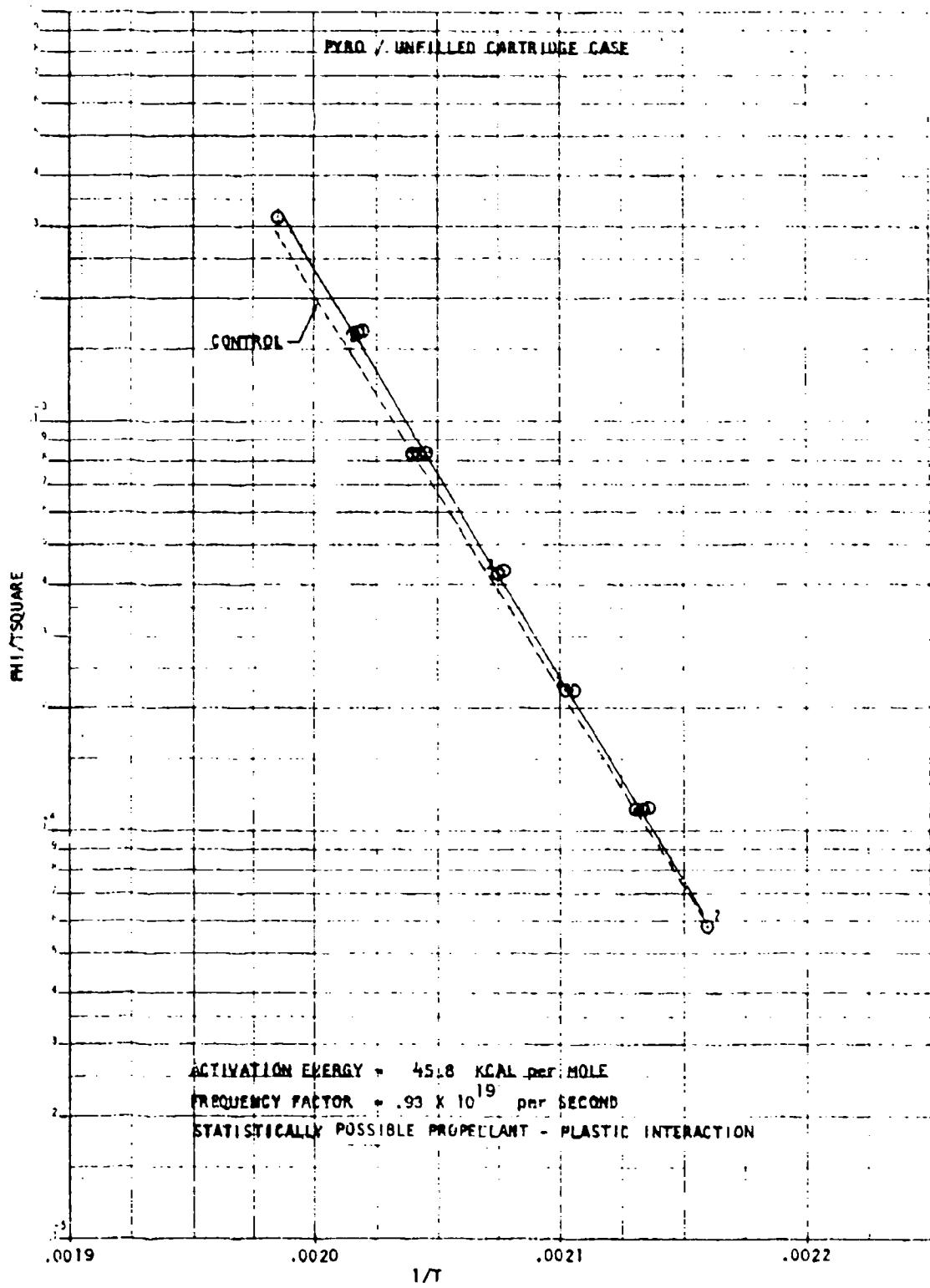
INPUT DATA

PHI	TEMP	1/T	PHI/TSQUARE
80.00	503.97	0.1984E-02	0.3150E-03
40.00	495.91	0.2016E-02	0.1627E-03
40.00	494.91	0.2021E-02	0.1633E-03
40.00	495.47	0.2018E-02	0.1629E-03
20.00	490.43	0.2039E-02	0.8315E-04
20.00	488.43	0.2047E-02	0.8383E-04
20.00	489.00	0.2045E-02	0.8364E-04
10.00	481.87	0.2075E-02	0.4307E-04
10.00	481.87	0.2075E-02	0.4307E-04
10.00	481.55	0.2077E-02	0.4312E-04
5.00	475.51	0.2103E-02	0.2211E-04
5.00	475.51	0.2103E-02	0.2211E-04
5.00	475.11	0.2105E-02	0.2215E-04
2.50	468.81	0.2133E-02	0.1137E-04
2.50	468.32	0.2135E-02	0.1140E-04
2.50	469.54	0.2130E-02	0.1134E-04
1.25	463.20	0.2159E-02	0.5826E-05
1.25	463.20	0.2159E-02	0.5826E-05

E (KCAL/MOLE) 0.457713E 02

A (SEC-1) 0.932722E 19

DEGREES KELVIN	K (SEC -1)	PERCENT, UNREACTED, (TIME IN YEARS)				
		1.0	2.0	5.0	10.0	20.0
298.0	0.25E-14	100.00	100.00	100.00	100.00	100.00
323.0	0.99E-12	100.00	99.99	99.98	99.97	99.94
348.0	0.17E-09	99.48	98.95	97.40	94.88	90.01
373.0	0.14E-07	64.12	41.11	10.84	1.17	0.01



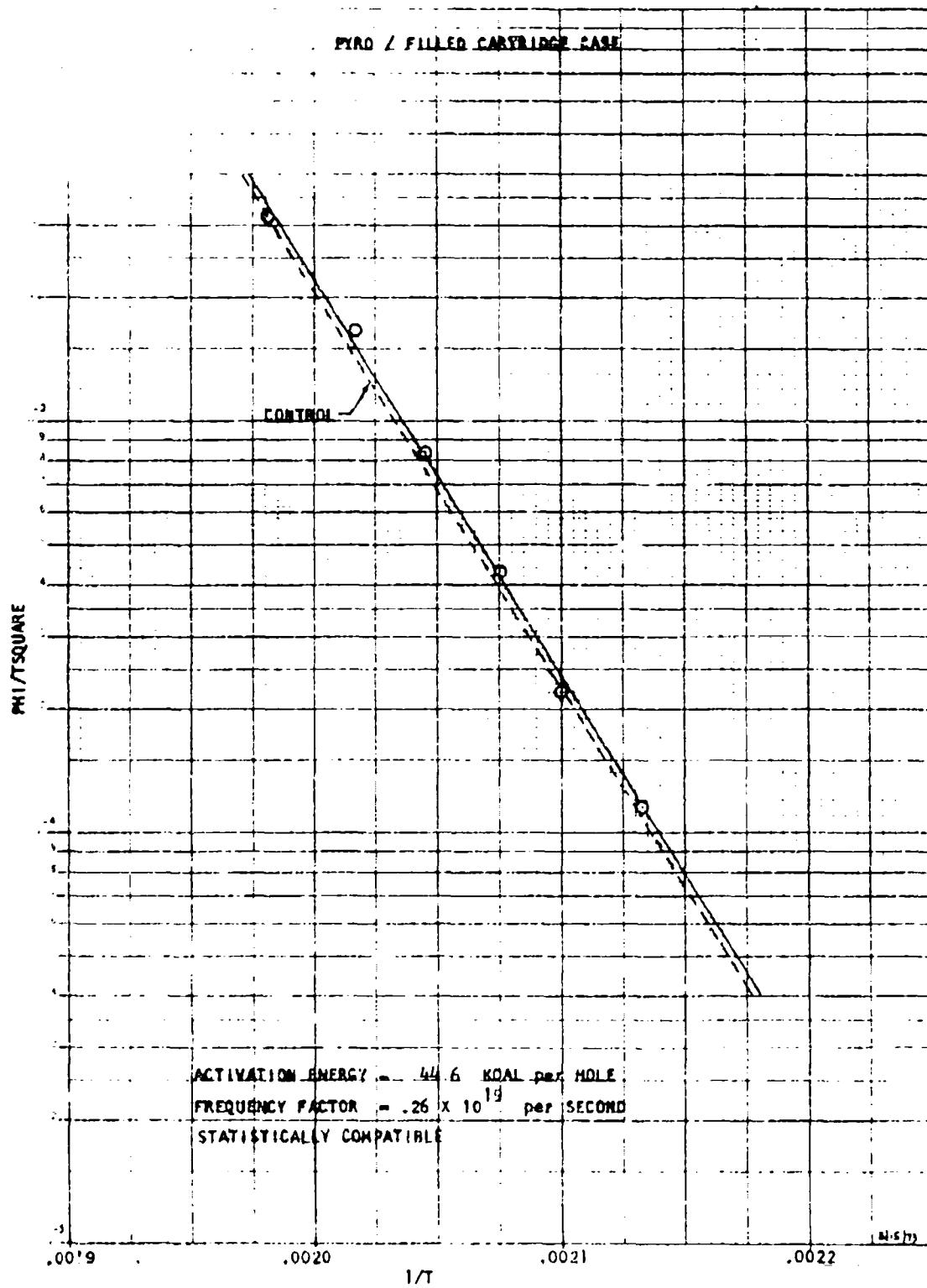
PYRO / FILLED CARTRIDGE CASE

INPUT DATA

PHI	I/TEMP	I/T	PHI/TSQUARE
80.00	504.67	0.1981E-02	0.3141E-03
40.00	495.67	0.2017E-02	0.1628E-03
20.00	489.00	0.2045E-02	0.8364E-04
10.00	482.04	0.2075E-02	0.4304E-04
5.00	476.19	0.2100E-02	0.2205E-04
2.50	468.85	0.2133E-02	0.1137E-04

E (KCAL/MOLE) 0.445877E 02
A (SEC-1) 0.253103E 19

DEGREES KELVIN	K (SEC -1)	PERCENT, UNREACTIONED, (TIME IN YEARS)				
		1.0	2.0	5.0	10.0	20.0
298.0	0.51E-14	100.00	100.00	100.00	100.00	100.00
323.0	0.17E-11	99.99	99.99	99.97	99.95	99.89
348.0	0.26E-09	99.20	98.40	96.05	92.25	85.11
373.0	0.19E-07	54.48	29.68	4.80	0.23	0.00



PYRO / ULTRABOND 76-125

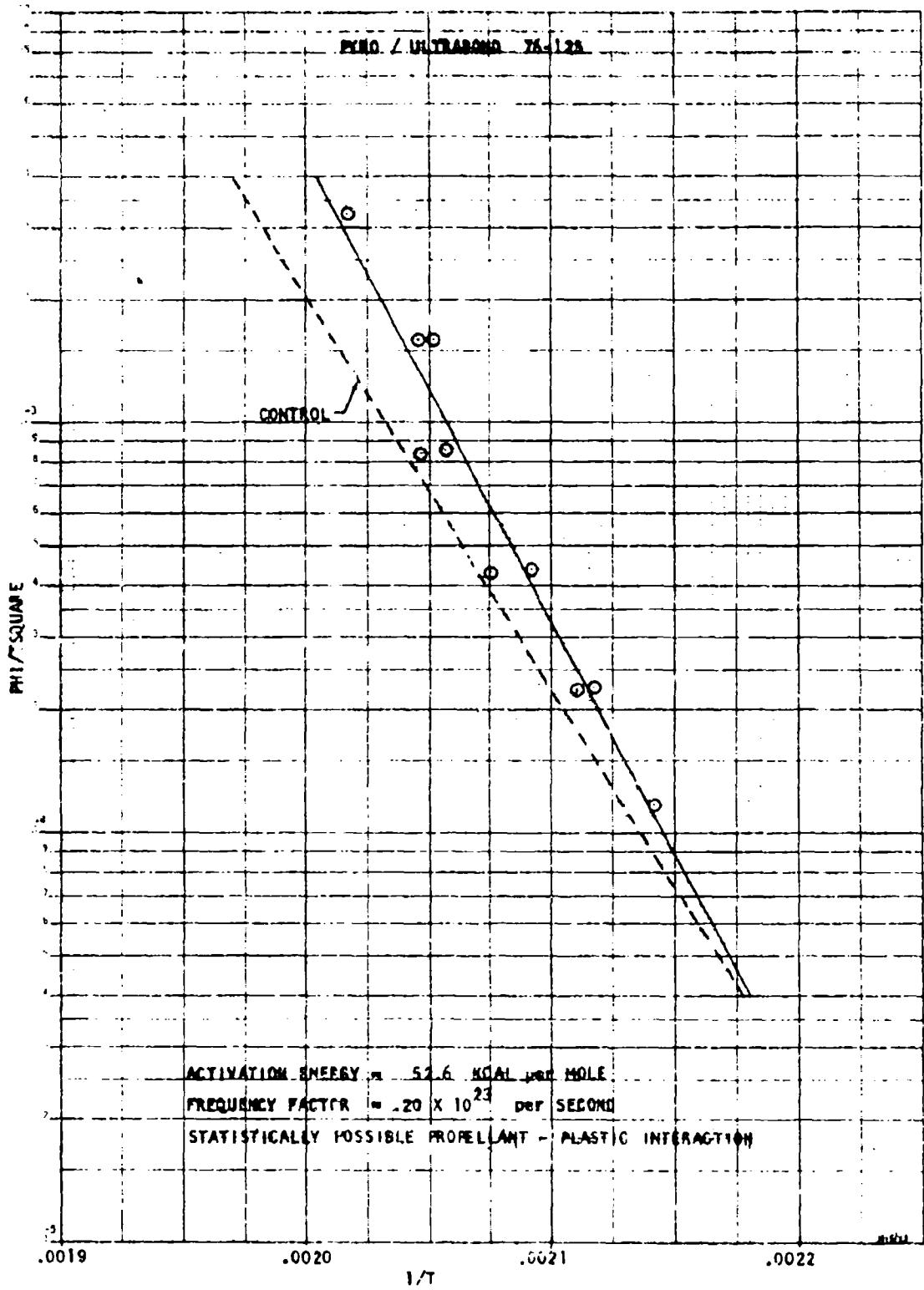
INPUT DATA

PHI	TEMP	1/T	PHI/TSQUARE
80.00	495.78	0.2017E-02	0.3255E-03
40.00	488.73	0.2046E-02	0.1675E-03
40.00	487.24	0.2052E-02	0.1685E-03
20.00	488.50	0.2047E-02	0.8381E-04
20.00	486.03	0.2057E-02	0.8466E-04
10.00	477.91	0.2092E-02	0.4378E-04
10.00	481.64	0.2076E-02	0.4311E-04
5.00	472.37	0.2117E-02	0.2241E-04
5.00	474.03	0.2110E-02	0.2225E-04
2.50	466.81	0.2142E-02	0.1117E-04

E (KCAL/MOLE) 0.526131E 02

A (SEC-1) 0.199368E 23

DEGREES KELVIN	K (SEC -1)	PERCENT, UNREACTED, (TIME IN YEARS)				
		1.0	2.0	5.0	10.0	20.0
293.0	0.51E-16	100.00	100.00	100.00	100.00	100.00
323.0	0.50E-13	100.00	100.00	100.00	100.00	100.00
348.0	0.18E-10	99.94	99.89	99.72	95.43	98.87
373.0	0.29E-08	91.12	83.02	62.80	39.4	15.56



PYRO / EC 1099

INPUT DATA

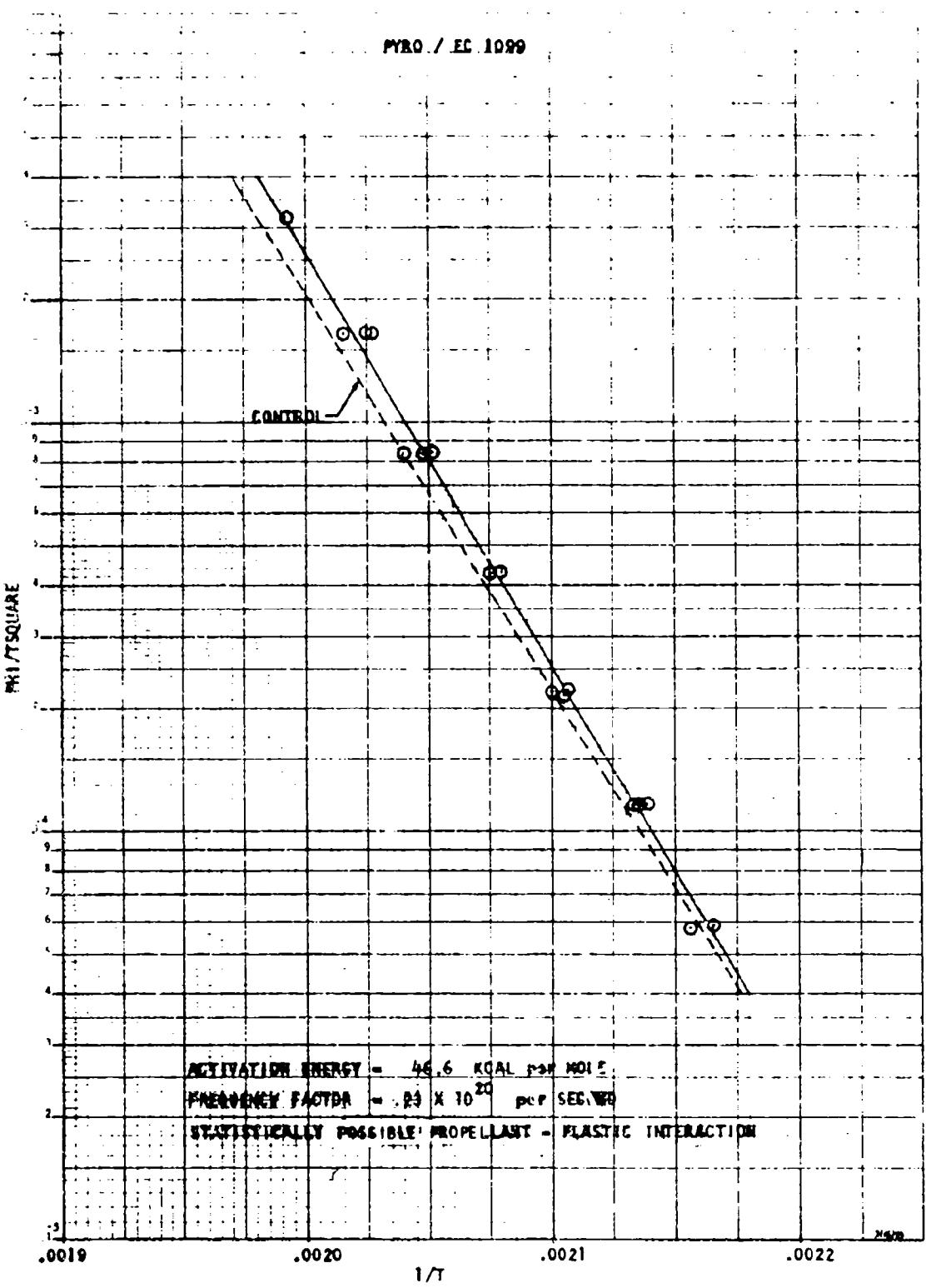
PH1	TEMP	1/T	PHI/ISQUARE
80.00	501.97	0.1992E-02	0.3175E-03
40.00	495.91	0.2016E-02	0.1627E-03
40.00	493.43	0.2027E-02	0.1643E-03
40.00	493.98	0.2024E-02	0.1639E-03
20.00	487.43	0.2052E-02	0.8418E-04
20.00	490.43	0.2039E-02	0.3015E-04
20.00	488.30	0.2048E-02	0.8389E-04
10.00	480.89	0.2079E-02	0.4324E-04
10.00	481.87	0.2075E-02	0.4307E-04
10.00	481.84	0.2075E-02	0.4307E-04
5.00	476.49	0.2099E-02	0.2202E-04
5.00	475.21	0.2104E-02	0.2214E-04
5.00	474.53	0.2107E-02	0.2220E-04
2.50	467.83	0.2138E-02	0.1142E-04
2.50	463.76	0.2133E-02	0.1138E-04
2.50	468.32	0.2135E-02	0.1140E-04
1.25	461.74	0.2166E-02	0.5863E-05
1.25	463.68	0.2157E-02	0.5814E-05

E (KCAL/MOLE) 0.465567E 02

A (SEC-1) 0.228539E 20

DEGREES K PERCENT, UNREACTED, (TIME IN YEARS)

KELVIN	K (SEC -1)	1.0	2.0	5.0	10.0	20.0
298.0	0.16E-14	100.00	100.00	100.00	100.00	100.00
323.0	0.72E-12	100.00	100.00	99.99	99.98	99.95
348.0	0.13E-09	99.59	99.18	97.95	95.94	92.05
373.0	0.12E-07	68.56	47.01	15.15	2.30	0.05



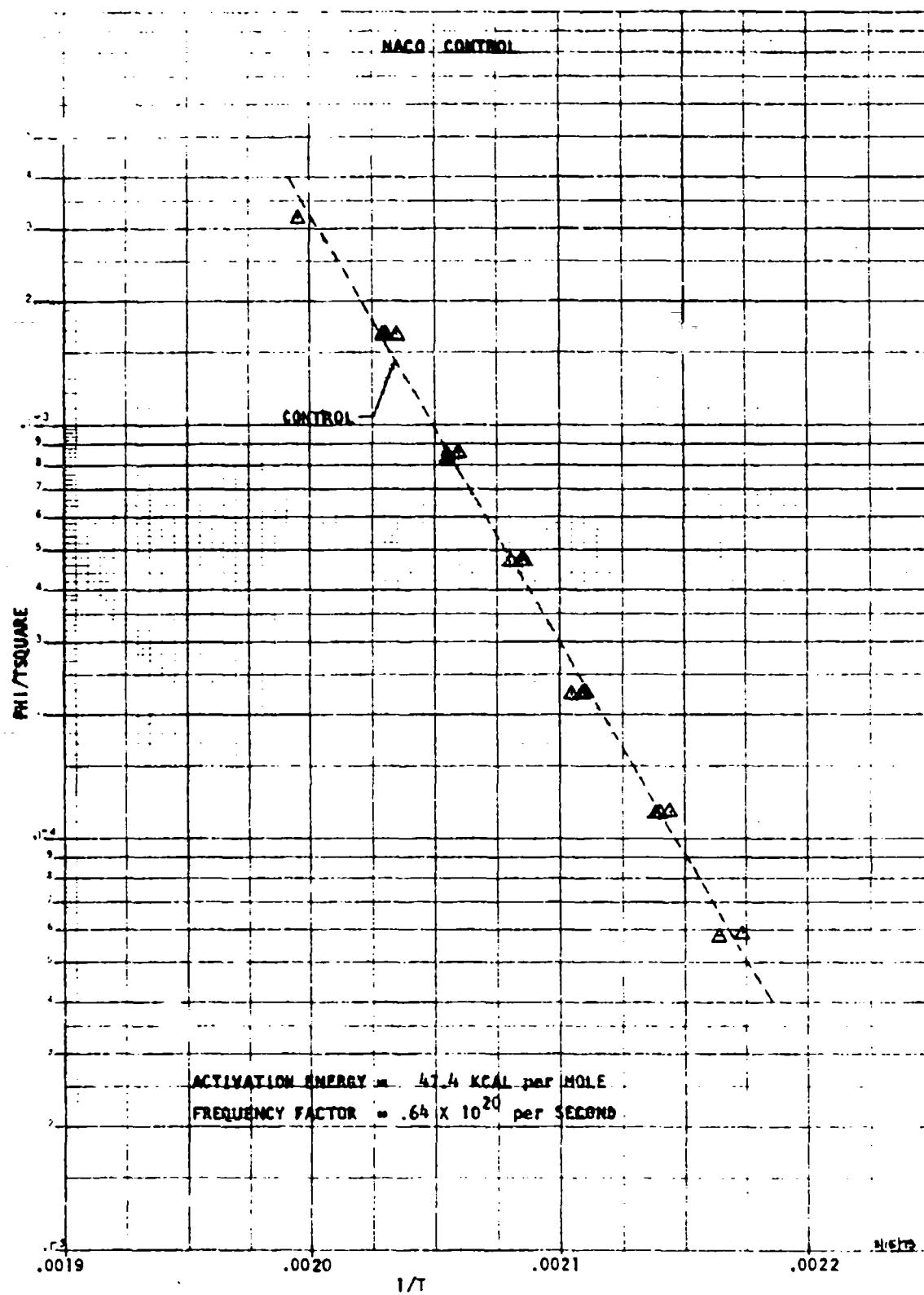
NACO CONTROL

INPUT DATA

PHI	TEMP	1/T	PHI/TSQUARE
80.00	501.27	0.1995E-02	0.3184E-03
40.00	492.44	0.2031E-02	0.1650E-03
40.00	492.93	0.2029E-02	0.1646E-03
40.00	491.70	0.2034E-02	0.1654E-03
20.00	486.44	0.2056E-02	0.8452E-04
20.00	485.44	0.2060E-02	0.8487E-04
20.00	486.72	0.2055E-02	0.8443E-04
10.00	479.90	0.2084E-02	0.4342E-04
10.00	479.41	0.2086E-02	0.4351E-04
10.00	480.86	0.2080E-02	0.4325E-04
5.00	474.04	0.2110E-02	0.2225E-04
5.00	475.02	0.2105E-02	0.2216E-04
5.00	473.64	0.2111E-02	0.2229E-04
2.50	466.37	0.2144E-02	0.1149E-04
2.50	467.64	0.2138E-02	0.1143E-04
2.50	467.39	0.2140E-02	0.1144E-04
1.25	460.29	0.2173E-02	0.5900E-05
1.25	462.23	0.2163E-02	0.5851E-05

E (KCAL/MOLE) 0.473649E 02
A (SEC-1) 0.643802E 20

DEGREES KELVIN	K (SEC -1)	PERCENT, UNREACTED, (TIME IN YEARS)				
		1.0	2.0	5.0	10.0	20.0
298.0	0.12E-14	100.00	100.00	100.00	100.00	100.00
323.0	0.57E-12	100.00	100.00	99.99	99.98	99.96
348.0	0.11E-09	99.64	99.28	98.20	96.44	93.01
373.0	0.11E-07	69.96	48.94	16.76	2.81	0.08



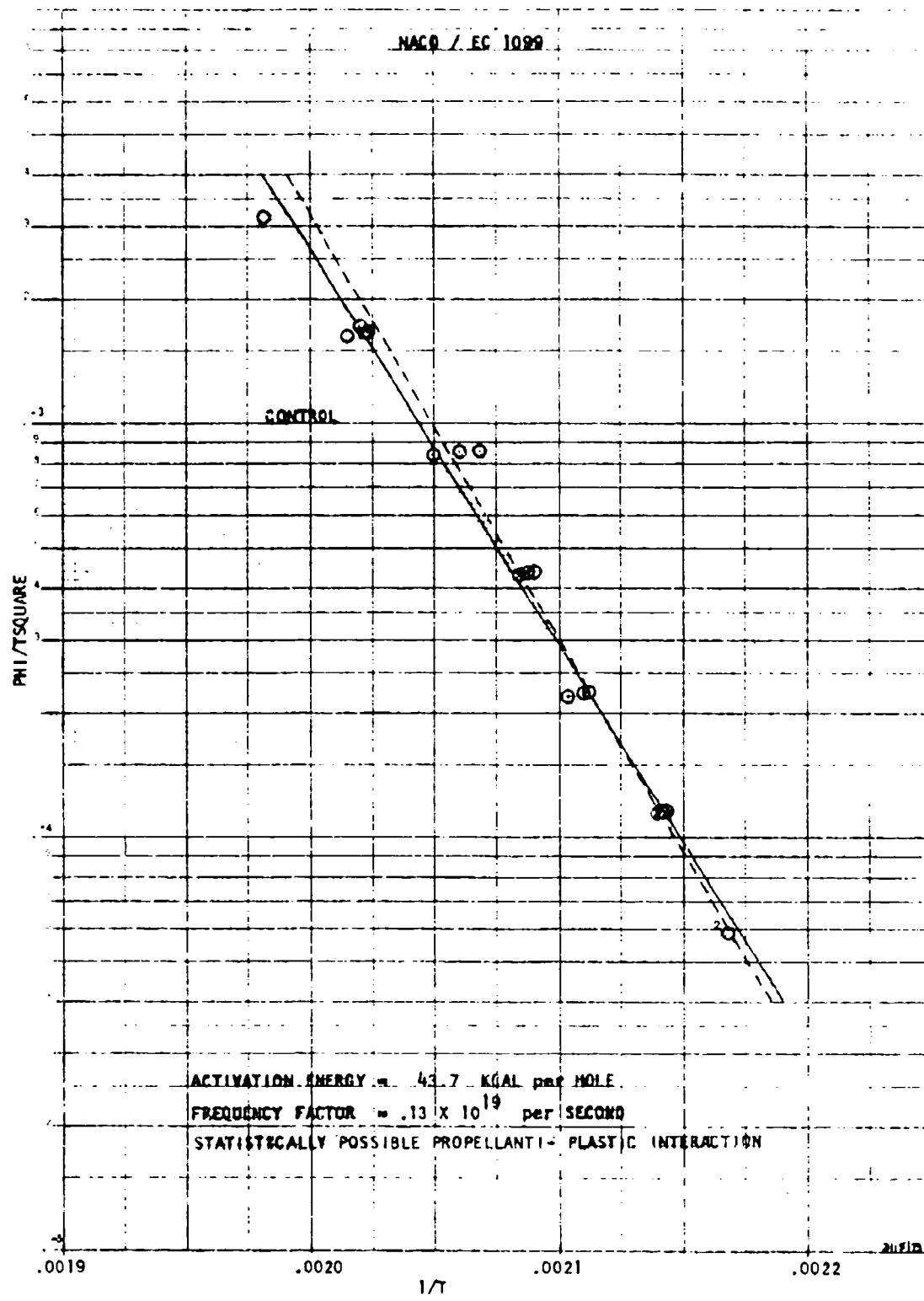
NACO / EC 1099

INPUT DATA

PHI	TEMP	1/T	PHI/ISQUARE
80.00	504.57	0.1982E-02	0.3142E-03
40.00	494.42	0.2023E-02	0.1636E-03
40.00	496.40	0.2015E-02	0.1623E-03
40.00	494.67	0.2022E-02	0.1635E-03
20.00	483.45	0.2068E-02	0.8557E-04
20.00	485.44	0.2060E-02	0.8487E-04
20.00	488.01	0.2049E-02	0.8398E-04
10.00	478.92	0.2088E-02	0.4360E-04
10.00	473.43	0.2090E-02	0.4369E-04
10.00	479.88	0.2084E-02	0.4342E-04
5.00	473.55	0.2112E-02	0.2230E-04
5.00	475.51	0.2103E-02	0.2211E-04
5.00	473.84	0.2110E-02	0.2227E-04
2.50	467.34	0.2140E-02	0.1145E-04
2.50	466.86	0.2142E-02	0.1147E-04
2.50	466.71	0.2143E-02	0.1148E-04
1.25	461.26	0.2168E-02	0.5875E-05
1.25	461.26	0.2168E-02	0.5875E-05

E (KCAL/MOLE) 0.437364E 02
 A (SEC-1) 0.126858E 19

DEGREES KELVIN	K (SEC -1)	PERCENT, UNREACTED, (TIME IN YEARS)				
		1.0	2.0	5.0	10.0	20.0
298.0	0.11E-13	100.00	100.00	100.00	100.00	100.00
323.0	0.32E-11	99.99	99.98	99.95	99.90	99.80
348.0	0.43E-09	98.65	97.32	93.44	87.31	76.23
373.0	0.30E-07	39.01	15.22	0.90	0.01	0.00



NACO / ULTRABOND 76-125

INPUT DATA

PHI	TEMP	I, I	PHI/ISQUARE
80.00	501.97	0.1992E-02	0.3175E-03
40.00	491.94	0.2033E-02	0.1653E-03
40.00	491.94	0.2033E-02	0.1653E-03
40.00	493.68	0.2026E-02	0.1641E-03
20.00	484.94	0.2062E-02	0.8505E-04
20.00	481.96	0.2075E-02	0.8610E-04
20.00	488.21	0.2048E-02	0.8391E-04
10.00	479.90	0.2084E-02	0.4342E-04
10.00	478.43	0.2090E-02	0.4369E-04
10.00	482.63	0.2072E-02	0.4293E-04
5.00	474.53	0.2107E-02	0.2220E-04
5.00	471.58	0.2121E-02	0.2248E-04
5.00	474.62	0.2107E-02	0.2220E-04
2.50	465.88	0.2146E-02	0.1152E-04
2.50	465.39	0.2149E-02	0.1154E-04
2.50	468.07	0.2136E-02	0.1141E-04
1.25	459.32	0.2177E-02	0.5925E-05
1.25	459.80	0.2175E-02	0.5913E-05

E (KCAL/MOLE) 0.446297E 02

A (SEC-1) 0.361088E 19

DEGREES K PERCENT, UNREACTED, (TIME IN YEARS)

KELVIN	(SEC -1)	1.0	2.0	5.0	10.0	20.0
298.0	0.67E-14	100.00	100.00	100.00	100.00	100.00
323.0	0.23E-11	99.99	99.99	99.96	99.93	99.86
348.0	0.34E-09	98.94	97.90	94.83	89.93	80.87
373.0	0.25E-07	44.81	20.08	1.81	0.03	0.00

